

Metabolomics Technologies for the Identification and Quantification of Dietary Phenolic Compound Metabolites: An Overview

Anallely López-Yerena ^{1,†}, Inés Domínguez-López ^{1,†}, Anna Vallverdú-Queralt ^{1,2}, Maria Pérez ^{1,3}, Olga Jáuregui ^{4,5}, Elvira Escribano-Ferrer ^{2,6,7,*} and Rosa M. Lamuela-Raventós ^{1,2,*}

¹ Department of Nutrition, Food Science and Gastronomy XaRTA, Institute of Nutrition and Food Safety (INSA-UB), Faculty of Pharmacy and Food Sciences, University of Barcelona, 08028 Barcelona, Spain; naye.yerena@gmail.com (A.L.-Y.); idinguez@ub.edu (I.D.-L.); avallverdu@ub.edu (A.V.-Q.); mariaperez@ub.edu (M.P.)

² CIBER Physiopathology of Obesity and Nutrition (CIBEROBN), Institute of Health Carlos III, 28029 Madrid, Spain

³ Laboratory of Organic Chemistry, Faculty of Pharmacy and Food Sciences, University of Barcelona, 08028 Barcelona, Spain

⁴ Scientific and Technological Center of University of Barcelona (CCiTUB), 08028 Barcelona, Spain; ojauregui@ccit.ub.edu

⁵ CIBER Fragilidad y Envejecimiento Saludable (CIBERfes), Instituto de Salud Carlos III, 28029, Madrid, Spain

⁶ Biopharmaceutics and Pharmacokinetics Unit, Department of Pharmacy and Pharmaceutical Technology and Physical Chemistry, Institute of Nanoscience and Nanotechnology (IN2UB), Faculty of Pharmacy and Food Sciences, University of Barcelona, 08028 Barcelona, Spain

⁷ Pharmaceutical Nanotechnology Group I+D+I Associated Unit to CSIC, University of Barcelona, 08028 Barcelona, Spain

† Equally Contributing Authors

* Correspondence: eescribano@ub.edu (E.E.-F.); lamuela@ub.edu (R.M.L.-R.); Tel.: +34-646421580 (R.M.L.-R.)

Table S1. Secoiridoids metabolites detected in plasma and/or urine from humans and rats.

| Food or supplement | Compounds | Metabolites | Parent mass | Fragments | Ref |
|--------------------|----------------------------|-----------------------------------|-------------|-----------|-------|
| EVOO | Oleuropein and/or oleacein | Hydroxytyrosol | 153 | 123 | [1,2] |
| | | Dihydroxyphenyl acetic acid | 167 | 123 | [1,3] |
| | | Hydroxytyrosol-glucuronide | 329 | 153 | [1] |
| | | Hydroxytyrosol-sulfate | 233 | 153 | [1,4] |
| | | Hydroxytyrosol acetate sulfate | 275 | 195 | [4] |
| | | Homovanillic acid | 181 | 137 | [1,3] |
| | | Homovanillic acid-glucuronide | 357 | 181 | [1] |
| | | Homovanillic alcohol | 167 | 152 | [1,3] |
| | | Homovanillic alcohol-sulfate | 247 | 167 | [1] |
| | | Elenolic acid | 241 | 139 | [1,3] |
| | | Elenolic acid-sulfate | 321 | 241 | |
| | | Elenolic acid-glucuronide | 417 | 241 | [1] |
| | | Methyloleuropein aglycone-sulfate | 471 | 391 | |
| | | Oleuropein aglycone-glucuronide | 553 | 377 | [5] |
| | | Oleacein | 319 | 195 | |
| | | Oleacein-sulfate | 399 | 319 | |
| | | Oleacein-glucuronide | 495 | 319/153 | |
| | Oleocanthal | Oleocanthal-hydrate | 319 | 153 | [7] |
| | | Oleocanthal-H ₂ O | 321 | 201 | |
| | | OLC-hydrate-glucuronide | 481 | 217 | |
| | | OLC-H ₂ O-glucuronide | 497 | 321 | |

EVOO: Extra virgin olive oil.

Table S2. Phenolic alcohol metabolites detected in plasma and/or urine from humans and rats.

| Food or supplement | Compounds | Metabolites | Parent mass | Fragments | Ref |
|--------------------|----------------|------------------------------------|-------------|-----------|-------------------|
| EVOO | Hydroxytyrosol | Hydroxytyrosol-glucuronide | 329 | 153 | [1,2,5,8–12] |
| | | Hydroxytyrosol-sulfate | 233 | 153/123 | [1,2,4–6,8,10–12] |
| | | Hydroxytyrosol acetate-sulfate | 275 | 195 | [4,5,10,12] |
| | | Hydroxytyrosol acetate-glucuronide | 371 | 195 | [5] |
| | | Homovanillic alcohol | 167 | 151/91 | [5,13] |
| | | Homovanillic alcohol-glucuronide | 343 | 167 | [5,9,10,12] |
| | | Homovanillic alcohol-sulfate | 247 | 167 | [5,10,12,13] |
| | | Homovanillic acid | 181 | 137 | [1,2,5,6] |
| | | Homovanillic acid-sulfate | 261 | 181 | [2,4–6,10–12] |
| | | Homovanillic acid-glucuronide | 357 | 181 | [5,12] |
| | | Hydroxytyrosol acetate | 195 | 91/123 | [5,13] |
| | | Dihydroxyphenylacetic acid | 169 | 123/110 | [13] |
| | | Tyrosol | 139* | 121/91 | |
| | Tyrosol | Tyrosol-glucuronide | 313 | 137 | [2,9] |
| | | Tyrosol-sulfate | 217 | 137 | [2,6,11] |

EVOO: Extra virgin olive oil. *In positive mode.

Table S3. Flavonoids metabolites detected in plasma and/or urine from humans and rats.

| Food or supplement | Compounds | Metabolites | Parent mass | Fragments | Ref |
|--|---------------|--|-------------|------------------------------|---------------------------|
| <i>Flavan-3-ols</i> | | | | | |
| Cocoa, cocoa drink, wine, grape extract or epicatechin standard | (Epi)catechin | (Epi)catechin | 289 | 245/205/179/137/151 | [14–19] |
| Black tea, cocoa, cocoa cream and drink, chocolate, dark chocolate, grape (extract and pomace drink), almond, (epi)catechin standard, polyphenol-rich juice, puree of (poly)phenol-rich berry fruits. | | (Epi)catechin-glucuronide | 465 | 289/245/205/179/203/289/245 | [15–29] |
| Cocoa drink, grape (pomace drink and extract, polyphenol-rich juice) | | (Epi)catechin-sulfate | 369 | 289/303/217/137/245 | [15–19,22–26,28–30] |
| (Epic)catechin standard | | (Epi)catechin-glucuronide-sulfate | 545 | 465/369/289 | [19,27,28,30] |
| Cocoa cream, catechin standard, Cocoa, cocoa drink, dark chocolate, chocolate, almond, grape extract, epicatechin standard, cranberry extract | | Methyl-(Epi)catechin | 305 | 179/147/139/137 | [18,20] |
| Cocoa cream, catechin standard Black tea, cocoa, cocoa cream and drink, chocolate, dark chocolate, grape (extract and pomace drink), almond, (epi)catechin standard, polyphenol-rich juice, puree of (poly)phenol-rich berry fruits. | | Methyl-(Epi)catechin-glucuronide | 479 | 179/139//137/303/289/175/461 | [15–21,24–26,31] |
| Cocoa drink, chocolate | | Methyl-(Epi)catechin-sulfate | 383 | 289/303/245/217/137 | [15,16,18–20,22,24–27,30] |
| Chocolate | | Methyl-(Epi)catechin-glucuronide-sulfate | 559 | 289 | [24,30] |
| Cranberry syrup | | Methyl-(Epi)catechin-diglucuronide-sulfate | 639 | 383 | [24] |
| Chocolate, epicatechin standard | | Catechin-hydrate | 287 | / | [32] |
| Epicatechin standard | | Catechin-hydrate-glucuronide | 463 | / | |
| Grape extract | | (Epi)catechin-glucoside | 451 | 289/313/161 | [18,24] |
| Polyphenol-rich juice | | (Epi)catechin-sulfate-glucoside | 531 | 369/289/451/313 | [18] |
| Black tea | | (Epi)gallocatechin | 305 | 225 | [19] |
| Grape extract, polyphenol-rich juice | | (Epi)gallocatechin-glucuronide | 481 | 305 | [28] |
| Almond, green tea | | Dimethyl-(Epi)gallocatechin-sulfate | 413 | / | [30] |
| Green tea, chocolate | | Methyl-epigallocatechin-glucuronide | 495 | 319 | [19,28] |
| Green tea, epicatechin standard, chocolate, almond | | Hydroxyphenyl- γ -valerolactone | 191 | 147 | [26,33] |
| Green tea, grape extract, epicatechin standard, chocolate, almond, concord grape juice | | Hydroxyphenyl- γ -valerolactone-glucuronide | 367 | 207/197/191 | [24,33] |
| Green tea, chocolate, almond, epicatechin standard | | Hydroxyphenyl- γ -valerolactone-sulfate | 271 | 191 | [18,24,26,33] |
| Green tea, epicatechin standard | | Dihydroxyphenyl- γ -valerolactone | 207 | 163/161/147/ 135/122/109 | [18,19,24,26,33,34] |
| | | Dihydroxyphenyl- γ -valerolactone-glucuronide | 383 | 207/175/163/135/122/113 | [24,26] |
| | | Dihydroxyphenyl- γ -valerolactone-sulfate | 287 | 207 | [18,33] |
| | | Dihydroxyphenyl- γ -valerolactone-di-sulfate | 367 | 287 | [33] |
| | | Trihydroxyphenyl- γ -valerolactone | 223 | 179 | |
| | | Methoxy-hydroxyphenyl- γ -valerolactone | 223 | 205/164/163 | [21] |

| | | | | | | | |
|--|---|---|--|-------------------------|---------------|------|----------------------------|
| Epicatechin standard | | Methoxy-hydroxyphenyl- γ -valerolactone-glucuronide | 399 | 381/223/205 | [18] | | |
| | | Methoxy-hydroxyphenyl- γ -valerolactone-sulfate | 303 | 285/223/163 | | | |
| | | Dihydroxyphenyl- γ -valeric acid-sulfate | 289 | 209/147/101 | | | |
| | | Trihydroxyphenyl- γ -valeric acid-sulfate | 305 | 225/207/123 | | | |
| | | Methyl-epicatechin-glucoside-sulfate | 545 | 383/303/245/327/501/217 | | | |
| Green tea, chocolate, almond, epicatechin standard | | Methoxyl-hydroxyphenyl- γ -valerolactone-glucuronide | 397 | 175/221/206/177/162/123 | [18,24,26,33] | | |
| Almond, epicatechin standard | | Methoxyl-hydroxyphenyl- γ -valerolactone-sulfate | 301 | 221 | [18,26] | | |
| Almond | | Hydroxyphenylpropionic acid | 165 | 121 | [26] | | |
| Epicatechin standard | | Hydroxyphenylpropionic acid-glucuronide | 341 | 175/165/121/113 | [18] | | |
| | | Hydroxyphenylpropionic acid-sulfate | 245 | 165/121 | | | |
| Almond | | Dihydroxyphenylpropionic acid | 181 | 137 | [26] | | |
| Epicatechin standard | | Methyl-dihydroxyphenylpropionic acid-sulfate | 275 | 195 | [18] | | |
| | | Dihydroxyphenylacetic acid-sulfate | 261 | 181/137/217 | | | |
| | | Hydroxyphenylacetic acid-sulfate | 231 | 151/217 | | | |
| | | Benzonic acid-sulfate | 217 | 137 | | | |
| | | Tetrahydroxyphenylpropanol-glucuronide | 451 | 275/217 | | | |
| | | Tetrahydroxyphenylpropanol-sulfate | 355 | 275 | | | |
| | | Pentahydroxyphenylpropanol-sulfate | 371 | 291/247/353/245 | | | |
| | | Methyl-pentahydroxyphenylpropanol-sulfate | 385 | 305 | | | |
| | | Methyl-pentahydroxyphenylpropanol-glucuronide | 481 | 305 | | | |
| | | Methyl-dihydroxyphenylacrylic acid-sulfate | 273 | 193/229 | | | |
| | Almond | Isorhamnetin | Isorhamnetin-glucuronide | 491 | | 315 | [26] |
| | | | Isorhamnetin-sulfate | 395 | | 315 | |
| | Green and black tea | | Methyl-epicatechin-sulfate | 383 | | / | [30,35] |
| Green tea, grape extract | | Epigallocatechin-glucuronide | 481 | 305 | [14,15,19] | | |
| Black tea | Epigallocatechin/ epicatechingallate/ epigallocatechingallate | Methyl-epigallocatechin-sulfate | 399 | / | [30] | | |
| | | Epicatechingallate-sulfate | 521 | / | | | |
| | | Epicatechingallate-glucuronide-sulfate | 697 | / | | | |
| | | Methyl-epicatechingallate-sulfate | 535 | / | | | |
| | | Methyl-epicatechingallate-glucuronide-sulfate | 711 | / | | | |
| | | Epigallocatechingallate-sulfate | 537 | / | | | |
| | | Methyl-epigallocatechingallate-sulfate | 551 | / | | [36] | |
| | | Black tea, yerba mate, orange juice, cranberry juice, strawberry, beans | Kaempferol | Kaempferol-glucuronide | | 461 | 363/285/257/229/175/113/85 |
| Wine | Phenylvalerolactones | Phenyl- γ -valerolactone-glucuronide | 367 | 191 | [42] | | |
| | | Phenyl- γ -valerolactone-sulfate | 271 | 191 | | | |
| Cocoa | Proanthocyanidin | Dihydroxyphenyl- γ -valerolactone | 207 | 163 | [15] | | |
| | | | Methoxy-hydroxyphenyl- γ -valerolactone | 221 | | 163 | |
| | Hydroxyphenyl-valerolactones | Dihydroxyphenyl- γ -valerolactone-glucuronide | 383 | 207 | | | |
| | | | Dihydroxyphenyl- γ -valerolactone-sulfate | 287 | | 207 | |
| | | | Methoxy-hydroxyphenyl- γ -valerolactone-glucuronide | 397 | | 221 | |
| Cocoa, chocolate | | Methoxy-hydroxyphenyl- γ -valerolactone-sulfate | 301 | 221/206/162/161/147 | [15,24] | | |
| Chocolate | | Methoxy-hydroxyphenyl- γ -valerolactone-sulfate | 317 | 222/179/163/137/125/113 | [24] | | |

| | | | | | |
|--|-----------------------|--|------------------|---------------------|---------------|
| | | Dihydroxyphenyl- γ -valerolactone-sulfate | 303 | 165/136/124/123/121 | |
| Cocoa, wine | | Procyanidin B1 | 577 | 425,289 | [14,42] |
| Wine | | Procyanidin B2 | 577 | 425, 289 | |
| Cranberry syrup | | Myricetin | 317 | / | [32] |
| | Myricetin | Methyl-myricetin | 331 | 317 | |
| | | Methyl-myricetin-glucuronide | 507 | 317 | |
| Tomato sauce, cranberry syrup, grape extract, beans | Quercetin | Quercetin | 301 | 151 | [19,32,41,43] |
| Tomato sauce, applesauce enriched with apple peel and onion, quercetin standard | | Quercetin-sulfate | 381 | 301/151 | [43–45] |
| Tomato sauce, cranberry (juice and syrup), applesauce enriched with apple peel and onion, quercetin standard | | Quercetin-glucuronide | 477 | 301/151 | [32,38,43–45] |
| Applesauce enriched with apple peel and onion, quercetin standard | | Quercetin-diglucuronide | 653 | 477/301 | [44,45] |
| | | Quercetin-glucuronide-sulfate | 557 | 477/380/301 | |
| Quercetin standard, cranberry syrup | | Methyl-quercetin | 315 | 300/151 | [32,44] |
| Yerba mate, applesauce enriched with apple peel and onion, quercetin standard, cranberry syrup | | Methyl-quercetin-glucuronide | 491 | 315/300 | [32,44–46] |
| Applesauce enriched with apple peel and onion or quercetin standard | | Methyl-quercetin-diglucuronide | 667 | 491/315/300 | [44,45] |
| Quercetin standard | | Methyl-quercetin-sulfate | 395 | 380/301 | [44] |
| | | Methyl-quercetin-glucuronide-sulfate | 571 | 491/315/301 | |
| | | Dimethyl-quercetin | 329 | 315/301 | |
| | | Dimethyl-quercetin-glucuronide | 505 | 491/315/301 | |
| Cranberry syrup | | Methoxy-quercetin-galactoside | 477 | / | [32] |
| Grape extract | Dihydroquercetin | 303 | 223 | [19] | |
| Applesauce enriched with apple peel and onion | Quercetin-glutathione | 651 | / | [45] | |
| Flavones | | | | | |
| EVOO | Apigenin | Apigenin-glucuronide | 445 | 269 | [6,11] |
| Luteolin standard | Luteolin | Luteolin-glucuronide | 461 | 285 | [47] |
| Isoflavones | | | | | |
| Daidzein standard | Daidzein | Equol | 241 | 212/135/121 | [48] |
| Daidzein standard, chocolate | | Equol-glucuronide | 417 | 175/241/113 | [48,49] |
| Chocolate | Equol | Equol-sulfate | 321 | 241 | [49] |
| Black soybean or daidzein standard | Daidzein | Genistein | 269 | 225/181/201 | [48,50] |
| Chocolate, black soybean | Genistein | Genistein-glucuronide | 445 | 269/175 | [49,50] |
| | | Genistein-sulfate | 349 | 269/303/225 | |
| Black soybean | | Hydroxygenistein-glucuronide | 461 | 286/175 | [50] |
| | | Daidzein | 253 | 225/209/197 | |
| Chocolate, black soybean, daidzein standard | Daidzein | Daidzein-glucuronide | 429 | 253/175 | [48–50] |
| | | Daidzein-sulfate | 333 | 253 | |
| | | Daidzein-disulfate | 413 | 333/253 | |
| Daidzein-glucuronide-sulfate | | 509 | 333/253 | | |
| Daidzein standard | | | Daidzein-hydrate | 255 | 135/254/149 |

| | | | | | |
|--|------------|----------------------------------|-----|---------------------------------|---------------|
| | | Daidzein-dihydrate | 257 | 137/161/147 | |
| | | Hydroge-daidzein-glucuronide | 431 | 255/175 | |
| Black soybean | | Hydroge-daidzein-sulfate | 335 | 255/253/207 | [50] |
| | | Methyl-daidzein | 267 | 252 | |
| Daidzein standard | | Daidzein-glucoside | 415 | 253/252/295 | [48] |
| | | Daidzin-glucoside | 579 | 2755/481 | |
| Black soybean, daidzein standard | | Daidzin | 415 | 253/191/155 | [48,50] |
| Black soybean | | Daidzin-sulfate | 495 | 415/253 | [50] |
| | | Puerarin | 415 | 295 | |
| | | Methyl-genistein | 283 | 268 | |
| | | Dimethyl-genistein | 285 | 270/149 | |
| | | Glucosygenistin | 593 | 269/431/433/271/178 | [48] |
| | | Hydroxygenistein | 285 | 257/229/217 | |
| Daidzein standard | | Hydroxygenistein-glucosides | 447 | 285/327/255 | |
| | | Glycitein | 283 | 268/240 | |
| | | Glycitein-glucuronide | 459 | 283/268/240 | [50] |
| | | Glycitein-sulfate | 363 | 283/268/240 | |
| | | Dihydroxyphenyl-chromane-diol | 275 | 151 | |
| | | Hydroxyphenyl-chromene-triol. | 271 | 165/151 | [48] |
| | | Hydroxyphenyl-chromen-ol | 239 | 147/195/197 | |
| Flavanones | | | | | |
| Tomato sauce, orange juice | | Naringenin | 271 | 253/235//151/119/107/93/83 | [37,43] |
| Tomato sauce, almond | | Naringenin-glucuronide | 447 | 271 | [26,43,51] |
| | | Naringenin-diglucuronide | 623 | 447/313/271/1757151/113 | [37,52] |
| | Naringenin | Naringenin-glucoside-glucuronide | 609 | 489/447/429/313/271/175/151/113 | |
| Orange juice | | Naringenin-glucoside-sulfate | 513 | 433/351/313/271/187/177/151/119 | |
| | | Naringenin-sulfate | 351 | 271/177/164/119/107/93 | [37] |
| | | Methylnaringenin-glucuronide | 461 | 285/270/243/175/164/151/113/85 | |
| Orange juice or hesperetin standard | | Hesperetin | 301 | 286/255/242/215/201/164/151/136 | [37,53] |
| Orange juice, polyphenol-rich juice, hesperetin standard | | Hesperetin-glucuronide | 477 | 301/175/151/459 | [28,37,52,53] |
| | | Hesperetin-diglucuronide | 653 | 477/301/286/242/175/113/85 | [37,52,53] |
| Orange juice, hesperetin standard | | Hesperetin-sulfate | 381 | 301/286/257/242/229/164/151/149 | [37,53] |
| | Hesperetin | Hesperetin-disulfate | 461 | 381/365/301/286/231/113 | [37] |
| Orange juice | | Hesperetin-glucuronide-sulfate | 557 | 477/381/301/286/254/242/229/113 | [28,37,52] |
| Orange juice, polyphenol-rich juice | | Hesperetin-glucoside | 463 | 175/445/151 | [53] |
| Hesperetin standard | | Hesperetin-sulfate-glucoside | 543 | 463/423/381/373/301/286/257/242 | [37] |
| | | Isosakuranetin-glucuronide | 461 | 285 | [52] |
| | | Dihsperetin-glucuronide | 955 | 477/301/175/113/85 | |
| | | Hesperidin | 609 | 301/286/257 | |
| Hesperidin standard | Hesperidin | Hesperidin-glucuronide | 477 | 301/459 | [37] |
| | | Hesperidin-sulfate | 381 | 229/149/134/151 | |
| | | Hesperidin-diglucuronide | 653 | 477/301 | |

| | | | | | |
|--------------------------------------|----------------------|----------------------------------|-----|---------------------------------|---------------|
| Orange juice | Eriodictyol | Hesperidin-glucoside | 611 | 413/197/443 | |
| | | Hesperidin-demethoxylate | 433 | 271/256/257//415 | |
| | | Hesperidin-demethylate | 595 | 577/559/529/487 | |
| | | Eriodictyol-glucuronide-sulfate | 543 | 463/367/287/254/187/175/151/135 | |
| | | Eriodictyol-glucuronide | 463 | 427/287/151/135/113/85 | |
| | | Eriodictyol-sulfate | 367 | 287/151/135/107 | |
| | | Homoeriodictyol | 301 | 286/242/201/174/151/136/108/107 | |
| Anthocyanidins | | | | | |
| Chokeberry extract, strawberry drink | Cyanidin | Cyanidin-glucoside | 449 | 287 | [36,39,54,55] |
| | | Cyanidin-glucuronide | 463 | 287 | [54] |
| Strawberry drink | Pelargonidin | Pelargonidin-glucuronide | 447 | / | |
| | | Pelargonidin-glucoside | 433 | 271/121 | [36,39,40] |
| | | Pelargonidin-rutinoside | 579 | 433/271 | |
| Bilberry | Peonidin-arabinoside | Delphinidin-glucuronide | 479 | 303 | |
| | Malvidin | Malvidin-arabinoside-glucuronide | 639 | 331 | |
| | Cyanidin | Peonidin-glucoside-glucuronide | 639 | 301 | |
| | Petunidin | Malvidin-glucoside-glucuronide | 669 | 339 | [56] |
| | Peonidin | Petunidin-glucoside-glucuronide | 655 | 317 | |
| Red raspberry | Anthocyanins | Hydroxybenzoic acid | 137 | 93 | |
| Red raspberry, yerba mate | | Hydroxybenzoic acid-sulfate | 233 | 153 | |
| | | Dihydroxybenzoic acid | 153 | 109 | [46,55] |
| Red raspberry | | Ferulic acid-glucuronide | 369 | 351/325/193/175/149/134/113/178 | |
| | | Hippuric acid | 178 | 134 | [55] |
| | | Hydroxyhippuric acid | 194 | 100/150 | |
| Almond | | Phenylacetic acid | 135 | 91 | |
| | | Hydroxyphenylacetic acid | 151 | 107 | [26] |
| Red raspberry, almond | | Dihydroxyphenylacetic acid | 167 | 123/137 | |
| | | Methoxy-hydroxyphenylacetic acid | 181 | 137/109/121 | [26,55] |
| | | Dihydrocaffeic acid-sulfate | 261 | 181/109/121 | |
| Red raspberry | | Ferulic acid | 193 | 134/178/149 | |
| | | Ferulic acid-glucuronide | 369 | 351/325/193/175/149/134/113/178 | [55] |
| | | Isoferulic acid-glucuronide | 369 | 193/178/113/134//175 | |
| | | Isoferulic acid-sulfate | 273 | 193/178/134/149 | |
| Cranberry extract | | Peonidin-glucoside | 461 | 264 | [31] |
| Dihydrochalcones | | | | | |
| Polyphenol-rich juice, apple | Phloretin | Phloretin-glucuronide | 449 | 273 | [28,57] |
| Polyphenol-rich juice | | Phloretin-glucuronide-sulfate | 529 | 353/449/273 | [28] |

Table S5. Metabolites of phenolic acids detected in plasma and/or urine from humans and rats.

| Food or supplement | Compounds | Metabolites | Parent mass | Fragments | Ref |
|---|---------------------|----------------------------------|-------------|----------------|--|
| <i>Hydroxybenzoic acids</i> | | | | | |
| Cocoa, EVOO, cranberry juice | | Vanillic acid | 167 | 152/123 | [6,14,15,38] |
| Orange juice, grape pomace drink, puree of (poly)phenol-rich berry fruits | | Vanillic acid-glucuronide | 343 | 167 | [27,29,52] |
| EVOO, orange juice, cranberry juice, grape pomace drink, puree of (poly)phenol-rich berry fruits, grape extract | | Vanillic acid-sulfate | 247 | 203, 167, 123 | [6,11,19,27,29,38,41,52] |
| Cranberry juice | | Isovanillic acid | 167 | / | [38] |
| Cocoa, grape extract, cranberry juice, almond, beans | | Protocatechuic acid | 153 | 109 | [14,15,19,26,38,41] |
| Grape extract | | Protocatechuic-glucoside | 315 | 153 | [19] |
| Grape pomace drink | Protocatechuic acid | Protocatechuic acid-glucuronide | 329 | 153 | [27] |
| Grape pomace, puree of (poly)phenol-rich berry fruits | | Protocatechuic acid-sulfate | 233 | 153 | [27,29] |
| Concord grape juice | Benzoic acid | Mandelic acid | 151 | 73 | [34] |
| | | Benzoic acid | 105 | 77 | |
| Grape pomace drink | | Benzoic acid-sulfate | 217 | 137 | [27] |
| Cocoa, coffee, beans, orange juice, red raspberry, strawberry, wine, cranberry (juice, syrup, and extract), almond, grape and concord grape juice | | Hydroxybenzoic acid | 137 | 93 | [14,15,19,26,27,31,32,32,34,36,38,41,42,52,58] |
| Coffee, cranberry juice, cranberry syrup | | Dihydroxybenzoic acid | 153 | 109 | [32,38,58] |
| Coffee, concord grape juice | | Methoxy-hydroxybenzoic acid | 167 | 123 | [34,58] |
| Tomato sauce, black tea, orange juice, wine, cranberry (juice and syrup), grape (extract, pomace drink, and juice) and beans | Benzoic acid | Hippuric acid | 178 | 134 | [19,27,30,32,34,38,41–43,52,59] |
| Almond, black tea, beans, cocoa, coffee, orange juice, tomato sauce, wine, yerba mate, cranberry (juice and syrup), and grape (extract, pomace drink, and juice). | Hydroxybenzoic acid | Hydroxyhippuric acid | 194 | 100 | [14,19,26,27,30,32,34,38,41–43,46,52,58,59] |
| Wine, cranberry juice, grape pomace drink. | | Gallic acid | 169 | 125 | [19,27,38] |
| Puree of (poly)phenol-rich berry fruits. | | Gallic acid-glucuronide | 345 | 169 | [29] |
| Grape extract, puree of (poly)phenol-rich berry fruits | | Methyl-gallic acid | 183 | 139/95 | [19,29] |
| Black tea, cranberry juice, grape extract, polyphenol-rich juice, puree of (poly)phenol-rich berry fruits | Gallic acid | Methyl-gallic acid-sulfate | 263 | 183 | [19,28–30,38] |
| Grape extract | | Dimethyl-gallic acid | 197 | 182/153/137 | [19] |
| Cranberry juice, grape extract | | Syringic acid | 197 | 137 | [19,38] |
| <i>Hydroxycinnamic acids</i> | | | | | |
| Cocoa, wine, cranberry juice, almond, coffee, beans, grape extract | Coumaric acid | Coumaric acid | 163 | 119/91 | [14,15,19,26,38,41,60] |
| Wine, coffee | | Coumaric acid-glucuronide | 339 | 163/113/119 | [42,58,60] |
| EVOO, coffee | | Coumaric acid-sulfate | 243 | 199/163/119 | [6,11,58,60,61] |
| Coffee, yerba mate | | Dihydrocoumaric acid | 165 | 121/106/59 | [46,58,60,62] |
| | | Dihydrocoumaric acid-glucuronide | 341 | 113/121/59/165 | [46,58,60] |

| | | | | | |
|---|---------------------------|---------------------------------|-----|---------------------------------|---|
| | | Dihydrocoumaric acid-sulfate | 245 | 165/121/59 | [46,58,60,62] |
| | | Dihydrocoumaroylquinic acid | 339 | 165 | [46,58] |
| Wine, cranberry syrup | | Coumaroyl-glucose | 325 | / | [32,63] |
| Coffee, yerba mate | | Coumaroylquinic acid | 337 | 163 | [46,58] |
| Cocoa, coffee, EVOO, tomato sauce, wine, grape extract, cranberry juice, almond, beans, standard solution | | Caffeic acid | 179 | 135 | [6,14,15,19,26,38,41–43,51,58,60,63,64] |
| Tomato sauce, coffee, yerba mate, grape extract, EVOO, polyphenol-rich juice, puree of (poly)phenol-rich berry fruits | Caffeic acid | Caffeic acid-sulfate | 259 | 215/179/135 | [6,19,28–30,43,58,60–62] |
| Tomato sauce, wine, cranberry juice, beans, standard solutions | | Caffeic acid-glucuronide | 355 | 311/179/135 | [38,41–43,51,60,61,64] |
| Cranberry syrup | | Caffeic acid-glucoside | 341 | 179 | [32] |
| | | Caffeic acid-glucoside hydrate | 339 | / | |
| Standard solution | | Hydroxyglucuronyl crylic acid | 355 | 337/311/293/179/175/135/113 | [64] |
| | | Glucuronylhydroxy crylic acid | 355 | 337/311/267/179/175/135/113 | |
| Tomato sauce, coffee, yerba mate, grape extract, cranberry juice | Caffeic acid | Dihydrocaffeic acid | 181 | 137/109 | [38,43,46,58,60,62] |
| Tomato sauce, coffee, yerba mate, cranberry juice, grape pomace drink, beans, polyphenol-rich juice | Dihydrocaffeic acid | Dihydrocaffeic acid-sulfate | 261 | 181/113 | [27,28,38,41,43,46,58,60,62] |
| Tomato sauce, coffee, yerba mate, grape extract, cranberry juice | | Dihydrocaffeic acid-glucuronide | 357 | 339/313/295/181/175/166/137/113 | [19,38,43,46,58,60,61] |
| Coffee, yerba mate | | Caffeoylquinic acid | 353 | 191/179 | [46,58,60,62] |
| Coffee | Caffeic acid | Caffeoylquinic-sulfate | 433 | 191/353/179 | [60] |
| | | Caffeoylquinic-lactone | 335 | 161/133 | |
| Coffee, yerba mate | | Dihydrocaffeoylquinic acid | 355 | 181 | [46,58] |
| Yerba mate | | Caffeoylquinic lactone-sulfate | 415 | 335 | [46] |
| Cocoa, tomato sauce, coffee, wine, cranberry juice, almond, standard solution | | Ferulic acid | 193 | 134/178/149 | [14,15,26,38,42,43,51,58,60,64] |
| Tomato sauce, coffee, yerba mate, orange juice, EVOO, cranberry juice, beans, polyphenol-rich juice, puree of (poly)phenol-rich berry fruits, grape extract | | Ferulic acid-sulfate | 273 | 193/149/134/178 | [6,19,28,29,38,41–43,46,52,58,60–62] |
| Tomato sauce, coffee, yerba mate, orange juice, EVOO, cranberry juice, grape pomace drink, puree of (poly)phenol-rich berry fruits | Undefined or ferulic acid | Ferulic acid-glucuronide | 369 | 351/325/193/175/149/134 | [6,27,29,38,41–43,46,51,52,58,60–62] |
| Coffee | Ferulic acid | Methyl-ferulic acid | 207 | 103/163 | [60,62] |
| | | Methyl-dihydroferulic acid | 209 | 150/165 | [60] |
| Yerba mate, cranberry juice, coffee, polyphenol-rich juice | | Dihydroferulic acid | 197 | 136 | [28,38,43,46,58,60,62] |
| Yerba mate, grape extract, cranberry (juice and syrup), coffee, beans | | Dihydroferulic acid-glucuronide | 373 | 195/175/136 | [19,32,38,41,43,46,60,62] |

| | | | | | | | | |
|--|-------------------------|--------------------------------------|-----|-----------------|------------------------------|--|--|--|
| Yerba mate, grape extract, coffee, orange juice, beans, (poly)phenol-rich berry fruits | | Dihydroferulic acid-sulfate | 277 | 195 | [19,28,38,41,43,46,52,60,62] | | | |
| Tomato sauce, coffee, yerba mate, cranberry juice, standard solution | | Isoferulic acid | 193 | 178/134 | [38,43,46,58,60,62,64] | | | |
| Coffee, yerba mate, orange juice, wine, cranberry juice, puree of (poly)phenol-rich berry fruits | | Isoferulic acid-glucuronide | 369 | 193/134 | [29,38,42,46,52,58,60,62] | | | |
| Coffee, yerba mate, polyphenol-rich juice | | Dihydroisoferulic acid | 195 | 136 | [28,46,58] | | | |
| Coffee, yerba mate, orange juice, cranberry juice, beans | | Dihydroisoferulic acid-glucuronide | 371 | 195/136 | [38,41,46,52,58] | | | |
| Coffee, yerba mate, EVOO, cranberry juice | | Dihydroisoferulic acid-sulfate | 273 | 195/136 | [11,38,46,58] | | | |
| Coffee, yerba mate | | Feruloylquinic acid | 367 | 191 | [46,58,60,62] | | | |
| Coffee | | Feruloylquinic-sulfate | 447 | 191/193 | [60] | | | |
| | | Feruloylquinic-glucuronide | 543 | 191/193 | | | | |
| | | Feruloylquinic-lactone | 349 | 175/160 | | | | |
| | | Dihydroferuloylquinic acid | 369 | 195 | | | | |
| Coffee, yerba mate | | Feruloylquinic lactone-glucuronide | 525 | 349 | [46,58] | | | |
| Coffee | | | | | [58] | | | |
| Coffee, yerba mate, orange juice, grape pomace drink, polyphenol-rich juice | | Feruloylglycine | 250 | 191/134 | [27,28,46,52,58] | | | |
| Coffee, yerba mate | | Isoferuloylglycine | 250 | 191/134 | [46,58] | | | |
| Cranberry juice, beans | | Sinapic acid | 223 | / | [38,41] | | | |
| Grape pomace drink | | Sinapic acid-sulfate | 303 | 223 | [27] | | | |
| Coffee | | Cinnamic acid | 147 | 103 | [60] | | | |
| | | Methoxy-cinnamic acid | 177 | 133/117 | | | | |
| | Dimethoxy-cinnamic acid | Dimethoxy-cinnamic acid | 207 | 103 | | | | |
| | | Dimethoxy-dihydrocinnamic acid | 209 | / | | | | |
| Almond | | Methoxy-hydroxycinnamic acid | 193 | 134 | [26] | | | |
| Tomato sauce, cranberry juice. | | Chlorogenic acid | 353 | 191 | [38,43] | | | |
| Cranberry syrup | | Hydroxychlorogenic acid | 369 | / | [32] | | | |
| | | Chlorogenic acid + H ₂ O | 371 | 353 | | | | |
| Coffee | Chlorogenic acid | Caffeoylquinic acid lactone-sulfate | 415 | 335/161/135 | [65] | | | |
| | | Feruloylquinic acid | 367 | 193 | | | | |
| | | Ferulic acid-sulfate | 273 | 193/178/149/134 | | | | |
| | | Feruloylglycine | 250 | 206/191/177/149 | | | | |
| | | Dihydroferulic acid-sulfate | 277 | 195/171/151 | | | | |
| | | Dihydroferulic acid-glucuronide | 371 | 195/173/113 | | | | |
| | | Isoferulic acid-sulfate | 273 | 193/178 | | | | |
| | | Isoferulic acid-glucuronide | 369 | 193/175/113 | | | | |
| | | Dihydro(iso)ferulic acid-glucuronide | 371 | 195/175/113 | | | | |
| | | Caffeic acid-sulfate | 259 | 179/135 | | | | |
| | | Dihydrocaffeic acid | 181 | 137/119 | | | | |
| | | Dihydrocaffeic acid-glucuronide | 357 | 181/175/137/113 | | | | |
| | | Dihydrocaffeic acid-sulfate | 261 | 181/137/119 | | | | |
| | | Hydroxyphenilacetic acids | | | | | | |

| | | | | | |
|--|--------------------------------|--|-------------------------------------|-----------------|---------------------------|
| Cocoa, coffee, wine, grape extract, cranberry juice, concord grape juice, wine | Hydroxyphenylacetic acid | Hydroxyphenylacetic acid | 151 | 107 | [14,15,19,34,38,38,42,58] |
| Tomato sauce | | Hydroxyphenylacetic acid-sulfate | 231 | 213/187/151/143 | [51] |
| Cocoa, yerba mate, coffee, grape extract, cranberry juice, concord grape juice | | Dihydroxyphenylacetic acid | 167 | 123/137 | [14,15,19,34,38,46,58] |
| Orange juice | | Dihydroxyphenylacetic acid-sulfate | 247 | 167 | [52] |
| Cocoa, yerba mate, wine, coffee, concord grape juice, wine | Dihydroxyphenylacetic acid | Methoxy-hydroxyphenylacetic acid | 181 | 137 | [14,15,34,34,42,46,58] |
| Black soybean | | Hydroxymethoxyl-phenylacetic acid-sulfate | 261 | 181/125 | [50] |
| Concord grape juice | | Phenoxyacetic acid | 151 | 165/147/135/73 | [34] |
| Cocoa, cranberry juice | | Phenylacetic acid | 135 | 91 | [14,15,38] |
| Grape extract, cranberry juice | | Homovanillic acid | 181 | 137 | [19,38] |
| Grape extract, beans, cranberry juice | | Homovanillic acid-sulfate | 261 | 181 | |
| Hydroxyphenylpropanoic acids | | | | | |
| Coffee | Phenylpropionic acid | Phenylpropionic acid | 149 | 105 | [60] |
| Wine | | Hydroxyphenylpropionic acid- sulfate | 245 | 165 | [42] |
| | | Hydroxyphenylpropionic acid-glucuronide | 341 | 165 | |
| Coffee | | Methoxy-phenylpropionic acid | 179 | 135 | [60] |
| | | Methoxy-hydroxyphenylpropionic acid-sulfate | 275 | 195 | [42] |
| Wine | | Methoxy-hydroxyphenylpropionic acid-glucuronide | 371 | 195 | |
| | | Wine, orange juice | Methoxy-hydroxyphenylpropionic acid | 195 | 136 |
| Tomato sauce, cocoa; yerba mate, wine, coffee, concord grape juice, cranberry juice, standard solution | | | Hydroxyphenylpropionic acid | 165 | 121 |
| Tomato sauce, wine, grape pomace drink | Hydroxyphenyl propionic acid | Hydroxyphenylpropionic acid-sulfate | 245 | 227/201/165/121 | [27,42] |
| Wine, orange juice | Dihydroxyphenylpropi onic acid | Dihydroxyphenylpropionic aci- glucuronide | 357 | 181 | [42,66] |
| Black tea | Homovanillic acid | Hydroxymethoxyphenylcarboxylic acid-sulfate | 261 | / | [30] |
| Cocoa, concord grape juice, cranberry juice, orange juice | | Dihydroxyphenylpropionic acid | 181 | 137 | [14,15,34,38,59] |
| Apple, orange juice | | Dihydroxyphenylpropionic acid-sulfate | 261 | 181 | [57,66] |
| Standard solution | | Dihydroxyphenylmethoxypropionic acid | 211 | 184/167/123 | [64] |
| | | Dihydroxyphenyllactic acid | 197 | 179/153/135/73 | |
| | | Trihydroxyphenyllactic acid | 213 | 195/169/151 | |
| | | Hydroxymethylphenyl lactic acid | 211 | 193/165/123 | |
| | | Hydroxymethyloxyphenyl lactic acid | 211 | 193/148/134 | |
| | | Dihydroxyphenyllactic acid methyl ester | 211 | 193/182/165/156 | |
| Hydroxyphenylpentanoic acids | | | | | |
| Cranberry juice, grape pomace drink, apple | | Phenyl- γ -valerolactone-sulfate | 271 | 191 | [27,67,68] |
| | | Phenyl- γ -valerolactone-glucuronide | 367 | 191 | |
| Grape pomace drink, apple | | Phenyl γ -valerolactone-glucuronide-sulfate | 463 | 287/207 | [27,68] |
| Cocoa | | Hydroxyphenyl- γ -valerolactone | 191 | 147 | [22] |
| Black tea, cocoa, cranberry extract | | Hydroxyphenyl- γ -valerolactone-sulfate | 271 | 191 | [22,30,31] |

| | | | | | |
|--|---|--|-----|-------------------|------------------|
| Black tea, cocoa | | Hydroxyphenyl- γ -valerolactone-glucuronide | 367 | 191 | [22,30] |
| Cocoa, cranberry juice, grape pomace drink | | Dihydroxyphenyl- γ -valerolactone | 207 | 163 | [22,27,67] |
| Cranberry juice, apple, grape pomace drink, black tea, cocoa | | Dihydroxyphenyl- γ -valerolactone-sulfate | 287 | 207 | [22,30,38,67,68] |
| Cranberry juice, grape pomace drink, apple, black tea | | Dihydroxyphenyl- γ -valerolactone-glucuronide | 383 | 207 | [27,30,67,68] |
| Black tea, cranberry juice, cocoa | | Dihydroxyphenyl γ -valerolactone-glucuronide-sulfate | 463 | 287 | [30,67] |
| | | Trihydroxy- γ -valerolactone-sulfate | 303 | / | |
| Black tea | Hydroxyphenyl- γ -valerolactone | Trihydroxy- γ -valerolactone-glucuronide | 399 | / | [30] |
| | | Trihydroxy- γ -valerolactone-glucuronide-sulfate | 479 | / | |
| | | Methyl-dihydroxyphenyl- γ -valerolactone-sulfate | 301 | 221 | [22] |
| Cocoa, black tea, cranberry juice | | Methyl-dihydroxyphenyl- γ -valerolactone-glucuronide | 397 | 221 | [22,30] |
| Cocoa, black tea | | Methyl-trihydroxyphenyl- γ -valerolactone-sulfate | 317 | / | [30] |
| Black tea | | Methyl-trihydroxyphenyl- γ -valerolactone-glucuronide | 413 | / | |
| Cranberry juice, grape pomace drink, apple | | Phenyl- γ -valerolactone-methoxy-sulfate | 301 | 221/206 | [27,67,68] |
| Cranberry juice, apple | | Phenyl- γ -valerolactone-methoxy-glucuronide | 397 | 221 | [67,68] |
| Chocolate, cranberry extract | | Dihydroxyphenylvaleric acid | 209 | 193/179/150/137 | [24,31] |
| Cocoa, chocolate | | Trihydroxyvaleric acid | 225 | 170/163/147/135 | [22,24] |
| Cranberry extract | | Dihydroxyvaleric acid-sulfate | 289 | / | [31] |
| Black tea, cocoa, chocolate, apple | | Trihydroxyvaleric acid-sulfate | 305 | 225/208/163/148 | [22,24,30,68] |
| | | Trihydroxyvaleric acid-glucuronide | 401 | 225/207/163/123 | |
| Black tea | Trihydroxyvaleric acid/ Tetrahydroxyvaleric acid | Methyl-dihydroxyphenylvaleric acid-sulfate | 303 | / | [30] |
| Black tea, chocolate | | Methyl-trihydroxyphenylvaleric acid-sulfate | 319 | 239/163/123/95/79 | [24,30] |
| Black tea | | Methyl-tetrahydroxyphenylvaleric acid-glucuronide | 431 | / | [30] |
| Apple | | Methoxy-hydroxyphenylvaleric acid-sulfate | 319 | 239 | [68] |

Table S5. Metabolites of enterolignans, stilbenes and ellagitannins detected in plasma and/or urine from humans and rats.

| Food or supplement | Compounds | Metabolites | Parent mass | Fragments | Ref |
|--|---------------|---|-------------|-----------------|------------|
| <i>Enterolignans</i> | | | | | |
| Cocoa | | Enterodiol | 301 | 253 | [14] |
| | | Enterolactone | 577 | 289 | |
| <i>Stilbenes</i> | | | | | |
| Wine, resveratrol pill and standard | Resveratrol | <i>trans</i> -/cis-resveratrol | 227 | 185 | [69–71] |
| Wine, grape extract, resveratrol pill and standard | | <i>trans</i> -/cis-resveratrol-glucuronide | 403 | 227 | [19,69–71] |
| | | <i>trans</i> -/cis-resveratrol-sulfate | 307 | 227 | |
| Resveratrol pill | | <i>trans</i> -resveratrol-glucuronide-sulfate | 483 | 307 | [71] |
| | | <i>trans</i> -resveratrol-diglucuronide | 579 | 403 | |
| Wine | | <i>trans</i> -/cis-piceid | 389 | 227 | [69] |
| | | <i>trans</i> -/cis-piceid-glucuronide | 565 | 389, 227 | |
| | | <i>trans</i> -/cis-piceid-sulfate | 469 | 389, 227 | |
| Wine, resveratrol pill | | Dihydroresveratrol | 229 | 123 | [69,71] |
| | | Dihydroresveratrol-glucuronide | 405 | 229 | |
| Wine, grape extract | | Dihydroresveratrol-sulfate | 309 | 229 | [19,69] |
| Grape extract, resveratrol pill | | Dihydroresveratrol-glucuronide sulfate | 485 | 309/ 233/ 175 | [19,71] |
| <i>Ellagitannins</i> | | | | | |
| Red raspberry | Ellagitannins | Urolithin A | 227 | 182/171 | [55] |
| | | Urolithin A-glucuronide | 403 | 175/171 | |
| | | Urolithin A-sulfate | 307 | 175/113 | |
| | | Isourolithin A-glucuronide | 403 | 171/175 | |
| | | (iso)Urolithin A-glucuronide-sulfate | 483 | 403/277/307/175 | |
| | | Urolithin B | 211 | 117/167 | |
| | | Urolithin B-glucuronide | 387 | 175/113 | |
| | | Dimethyllellagic acid-glucuronide | 505 | 113/175 | |

Table S6. Metabolites of other phenolic compounds detected in plasma and/or urine from humans and rats.

| Food or supplement | Compounds | Metabolites | Parent mass | Fragments | Ref |
|--|------------|---|-------------|-----------|---------------------|
| Wine, concord grape juice | | Tartaric acid | 149 | / | [34,63] |
| Wine | | Ethyl hydrogen-sulfate | 125 | / | [63] |
| | | Monoglyceride citrate | 265 | / | |
| | | Galactosylglycerol | 253 | / | |
| | | Methylisocitric acid | 187 | / | |
| | | Isopropyl-oxosuccinate | 219 | / | |
| | | Dihydroxy-methoxyacetophenone-glucoside | 343 | / | [42,63] |
| | | Ethyl maltol | 139 | / | |
| | | Phloroglucinol | 125 | / | |
| | | α -terpinyl cinnamate | 283 | / | |
| | | Licarin C/kanzonol R | 369 | / | |
| | | Kanzonol I | 435 | / | [63] |
| Grape extract, concord grape juice | | Pyrogallol | 125 | 97 | [19,34] |
| Black tea, cranberry juice, beans, puree of (poly)phenol-rich berry fruits | Pyrogallol | Pyrogallol-sulfate | 204 | 125 | [29,30,38,41] |
| Cranberry juice, grape pomace drink, beans, puree of (poly)phenol-rich berry fruits | | Methylpyrogallol-sulfate | 218 | 139, 124 | [29] |
| Black tea, puree of (poly)phenol-rich berry fruits | | Pyrogallol-glucuronide | 301 | 125 | [29,30] |
| Black tea | Pyrogallol | Dihydroxyphenyl-sulfate | 209 | 129 | [72] |
| Grape extract | | Methylpyrogallol | 139 | 124 | [29] |
| Cranberry (juice and extract), grape pomace drink, beans, puree of (poly)phenol-rich berry fruits, apple | | Catechol-sulfate | 189 | 109 | [27,29,31,38,41,57] |
| Puree of (poly)phenol-rich berry fruits | | Catechol-glucuronide | 285 | | [29] |
| Cranberry juice, grape pomace drink, beans, puree of (poly)phenol-rich berry fruits, apple | | Methylcatechol-sulfate | 203 | 123 | [27,29,38,41,57] |
| Puree of (poly)phenol-rich berry fruits | | Methylcatechol-glucuronide | 299 | | [29] |
| Black tea | Resorcinol | Diphenol-glucuronide | 285 | / | [30] |
| | | Diphenol-sulfate | 188 | / | |
| Cranberry juice, beans | | Hydroxybenzaldehyde | 121 | / | [38,41] |
| Cranberry juice | | Dihydroxybenzaldehyde | 137 | / | [38] |
| EVOO, almond | | Vanillin | 151 | 136 | [6,26] |
| EVOO | | Vanillin-sulfate | 231 | 151/136 | [6] |
| | | Vanillin-glucuronide | 327 | | |
| | | Scopoletin | 193 | / | |
| Cranberry syrup | | Methyl-scopoletin | 207 | / | [32] |
| | | Dihydroxycoumarin-glucuronide | 355 | / | |
| | | Methyl-hydroxycoumarin-glucuronide | 353 | / | |
| | | | | | |

References

- [1] M.-C. López de las Hazas, C. Piñol, A. Macià, M.-P. Romero, A. Pedret, R. Solà, L. Rubió, M.-J. Motilva, Differential absorption and metabolism of hydroxytyrosol and its precursors oleuropein and secoiridoids, *Journal of Functional Foods*. 22 (2016) 52–63. <https://doi.org/10.1016/j.jff.2016.01.030>.
- [2] M.I. Orozco-Solano, C. Ferreira-Vera, F. Priego-Capote, M.D. Luque de Castro, Automated method for determination of olive oil phenols and metabolites in human plasma and application in intervention studies, *Journal of Chromatography A*. 1258 (2012) 108–116. <https://doi.org/10.1016/j.chroma.2012.08.057>.
- [3] F.N. Bazoti, E. Gikas, A. Tsarbopoulos, Simultaneous quantification of oleuropein and its metabolites in rat plasma by liquid chromatography electrospray ionization tandem mass spectrometry, *Biomed. Chromatogr.* 24 (2010) 506–515. <https://doi.org/10.1002/bmc.1319>.
- [4] L. Rubió, R.-M. Valls, A. Macià, A. Pedret, M. Giralt, M.-P. Romero, R. de la Torre, M.-I. Covas, R. Solà, M.-J. Motilva, Impact of olive oil phenolic concentration on human plasmatic phenolic metabolites, *Food Chemistry*. 135 (2012) 2922–2929. <https://doi.org/10.1016/j.foodchem.2012.07.085>.
- [5] L. Rubió, A. Macià, R.M. Valls, A. Pedret, M.-P. Romero, R. Solà, M.-J. Motilva, A new hydroxytyrosol metabolite identified in human plasma: Hydroxytyrosol acetate sulphate, *Food Chemistry*. 134 (2012) 1132–1136. <https://doi.org/10.1016/j.foodchem.2012.02.192>.
- [6] M. Suárez, R.M. Valls, M.-P. Romero, A. Macià, S. Fernández, M. Giralt, R. Solà, M.-J. Motilva, Bioavailability of phenols from a phenol-enriched olive oil, *Br J Nutr.* 106 (2011) 1691–1701. <https://doi.org/10.1017/S0007114511002200>.
- [7] López-Yerena, Vallverdú-Queralt, Mols, Augustijns, Lamuela-Raventós, Escribano-Ferrer, Absorption and Intestinal Metabolic Profile of Oleocanthal in Rats, *Pharmaceutics*. 12 (2020) 134. <https://doi.org/10.3390/pharmaceutics12020134>.
- [8] O. Khymenets, M.C. Crespo, O. Dangles, N. Rakotomanomana, C. Andres-Lacueva, F. Visioli, Human hydroxytyrosol's absorption and excretion from a nutraceutical, *Journal of Functional Foods*. 23 (2016) 278–282. <https://doi.org/10.1016/j.jff.2016.02.046>.
- [9] O. Khymenets, M. Farré, M. Pujadas, E. Ortiz, J. Joglar, M.I. Covas, R. de la Torre, Direct analysis of glucuronidated metabolites of main olive oil phenols in human urine after dietary consumption of virgin olive oil, *Food Chemistry*. 126 (2011) 306–314. <https://doi.org/10.1016/j.foodchem.2010.10.044>.
- [10] A. Serra, L. Rubió, A. Macià, R.-M. Valls, Ú. Catalán, Application of dried spot cards as a rapid sample treatment method for determining hydroxytyrosol metabolites in human urine samples. Comparison with microelution solid-phase extraction, (n.d.) 14.
- [11] M. Suárez, M.-P. Romero, A. Macià, R.M. Valls, S. Fernández, R. Solà, M.-J. Motilva, Improved method for identifying and quantifying olive oil phenolic compounds and their metabolites in human plasma by microelution solid-phase extraction plate and liquid chromatography–tandem mass spectrometry, *Journal of Chromatography B*. 877 (2009) 4097–4106. <https://doi.org/10.1016/j.jchromb.2009.10.025>.
- [12] M.-C. López de las Hazas, L. Rubió, A. Kotronoulas, R. de la Torre, R. Solà, M.-J. Motilva, Dose effect on the uptake and accumulation of hydroxytyrosol and its metabolites in target tissues in rats, *Mol. Nutr. Food Res.* 59 (2015) 1395–1399. <https://doi.org/10.1002/mnfr.201500048>.
- [13] R. Domínguez-Perles, D. Auñón, F. Ferreres, A. Gil-Izquierdo, Gender differences in plasma and urine metabolites from Sprague–Dawley rats after oral administration of normal and high doses of hydroxytyrosol, hydroxytyrosol acetate, and DOPAC, *Eur J Nutr.* 56 (2017) 215–224. <https://doi.org/10.1007/s00394-015-1071-2>.
- [14] M. Urpi-Sarda, M. Monagas, N. Khan, R.M. Lamuela-Raventós, C. Santos-Buelga, E. Sacanella, M. Castell, J. Permanyer, C. Andres-Lacueva, Epicatechin, procyanidins, and

- phenolic microbial metabolites after cocoa intake in humans and rats, *Anal Bioanal Chem.* 394 (2009) 1545–1556. <https://doi.org/10.1007/s00216-009-2676-1>.
- [15] M. Urpi-Sarda, M. Monagas, N. Khan, R. Llorach, R.M. Lamuela-Raventós, O. Jáuregui, R. Estruch, M. Izquierdo-Pulido, C. Andrés-Lacueva, Targeted metabolic profiling of phenolics in urine and plasma after regular consumption of cocoa by liquid chromatography–tandem mass spectrometry, *Journal of Chromatography A.* 1216 (2009) 7258–7267. <https://doi.org/10.1016/j.chroma.2009.07.058>.
- [16] E. Roura, C. Andrés-Lacueva, O. Jáuregui, E. Badia, R. Estruch, M. Izquierdo-Pulido, R.M. Lamuela-Raventós, Rapid Liquid Chromatography Tandem Mass Spectrometry Assay To Quantify Plasma (–)-Epicatechin Metabolites after Ingestion of a Standard Portion of Cocoa Beverage in Humans, *J. Agric. Food Chem.* 53 (2005) 6190–6194. <https://doi.org/10.1021/jf050377u>.
- [17] J.I. Ottaviani, T.Y. Momma, G.K. Kuhnle, C.L. Keen, H. Schroeter, Structurally related (–)-epicatechin metabolites in humans: Assessment using de novo chemically synthesized authentic standards, 52 (2012) 1403–1412. <https://doi.org/10.1016/j.freeradbiomed.2011.12.010>.
- [18] Z. Shang, F. Wang, S. Dai, J. Lu, X. Wu, J. Zhang, Profiling and identification of (–)-epicatechin metabolites in rats using ultra-high performance liquid chromatography coupled with linear trap-Orbitrap mass spectrometer: Study of EC in vivo metabolites, *Drug Test. Analysis.* 9 (2017) 1224–1235. <https://doi.org/10.1002/dta.2155>.
- [19] G. Sasot, M. Martínez-Huélamo, A. Vallverdú-Queralt, M. Mercader-Martí, R. Estruch, R.M. Lamuela-Raventós, Identification of phenolic metabolites in human urine after the intake of a functional food made from grape extract by a high resolution LTQ-Orbitrap-MS approach, *Food Research International.* 100 (2017) 435–444. <https://doi.org/10.1016/j.foodres.2017.01.020>.
- [20] A. Serra, A. Macià, L. Rubió, N. Anglès, N. Ortega, J.R. Morelló, M.-P. Romero, M.-J. Motilva, Distribution of procyanidins and their metabolites in rat plasma and tissues in relation to ingestion of procyanidin-enriched or procyanidin-rich cocoa creams, *Eur J Nutr.* 52 (2013) 1029–1038. <https://doi.org/10.1007/s00394-012-0409-2>.
- [21] A. Fardet, R. Llorach, J.-F. Martin, C. Besson, B. Lyan, E. Pujos-Guillot, A. Scalbert, A Liquid Chromatography–Quadrupole Time-of-Flight (LC–QTOF)-based Metabolomic Approach Reveals New Metabolic Effects of Catechin in Rats Fed High-Fat Diets, *J. Proteome Res.* 7 (2008) 2388–2398. <https://doi.org/10.1021/pr800034h>.
- [22] M. Gómez-Juaristi, B. Sarria, S. Martínez-López, L. Bravo Clemente, R. Mateos, Flavanol Bioavailability in Two Cocoa Products with Different Phenolic Content. A Comparative Study in Humans, *Nutrients.* 11 (2019) 1441. <https://doi.org/10.3390/nu11071441>.
- [23] E. Roura, C. Andrés-Lacueva, R. Estruch, M. Lourdes Mata Bilbao, M. Izquierdo-Pulido, R.M. Lamuela-Raventós, The effects of milk as a food matrix for polyphenols on the excretion profile of cocoa (–)-epicatechin metabolites in healthy human subjects, *Br J Nutr.* 100 (2008) 846–851. <https://doi.org/10.1017/S0007114508922534>.
- [24] I. Hakeem Said, J.D. Truex, C. Heidorn, M.B. Retta, D.D. Petrov, S. Haka, N. Kuhnert, LC-MS/MS based molecular networking approach for the identification of cocoa phenolic metabolites in human urine, *Food Research International.* 132 (2020) 109119. <https://doi.org/10.1016/j.foodres.2020.109119>.
- [25] L. Actis-Goretta, A. Lévêques, F. Giuffrida, F. Romanov-Michailidis, F. Viton, D. Barron, M. Duenas-Paton, S. Gonzalez-Manzano, C. Santos-Buelga, G. Williamson, F. Dionisi, Elucidation of (–)-epicatechin metabolites after ingestion of chocolate by healthy humans, *Free Radical Biology and Medicine.* 53 (2012) 787–795. <https://doi.org/10.1016/j.freeradbiomed.2012.05.023>.
- [26] M. Urpi-Sarda, I. Garrido, M. Monagas, C. Gómez-Cordovés, A. Medina-Remón, C. Andres-Lacueva, B. Bartolomé, Profile of Plasma and Urine Metabolites after the Intake of Almond

- [Prunus dulcis (Mill.) D.A. Webb] Polyphenols in Humans, *J. Agric. Food Chem.* 57 (2009) 10134–10142. <https://doi.org/10.1021/jf901450z>.
- [27] F. Castello, G. Costabile, L. Bresciani, M. Tassotti, D. Naviglio, D. Luongo, P. Ciciola, M. Vitale, C. Vetrani, G. Galaverna, F. Brighenti, R. Giacco, D. Del Rio, P. Mena, Bioavailability and pharmacokinetic profile of grape pomace phenolic compounds in humans, *Archives of Biochemistry and Biophysics*. 646 (2018) 1–9. <https://doi.org/10.1016/j.abb.2018.03.021>.
- [28] W. Mullen, G. Borges, M.E.J. Lean, S.A. Roberts, A. Crozier, Identification of Metabolites in Human Plasma and Urine after Consumption of a Polyphenol-Rich Juice Drink, *J. Agric. Food Chem.* 58 (2010) 2586–2595. <https://doi.org/10.1021/jf904096v>.
- [29] R.C. Pimpão, T. Dew, M.E. Figueira, G.J. McDougall, D. Stewart, R.B. Ferreira, C.N. Santos, G. Williamson, Urinary metabolite profiling identifies novel colonic metabolites and conjugates of phenolics in healthy volunteers, *Mol. Nutr. Food Res.* 58 (2014) 1414–1425. <https://doi.org/10.1002/mnfr.201300822>.
- [30] J. van Duynhoven, J.J.J. van der Hooft, F.A. van Dorsten, S. Peters, M. Foltz, V. Gomez-Roldan, J. Vervoort, R.C.H. de Vos, D.M. Jacobs, Rapid and Sustained Systemic Circulation of Conjugated Gut Microbial Catabolites after Single-Dose Black Tea Extract Consumption, *J. Proteome Res.* 13 (2014) 2668–2678. <https://doi.org/10.1021/pr5001253>.
- [31] H. Liu, T.J. Garrett, F. Tayyari, L. Gu, Profiling the metabolome changes caused by cranberry procyanidins in plasma of female rats using ¹ H NMR and UHPLC-Q-Orbitrap-HRMS global metabolomics approaches, *Mol. Nutr. Food Res.* 59 (2015) 2107–2118. <https://doi.org/10.1002/mnfr.201500236>.
- [32] I. Iswaldi, D. Arráez-Román, A.M. Gómez-Caravaca, M. del M. Contreras, J. Uberos, A. Segura-Carretero, A. Fernández-Gutiérrez, Identification of polyphenols and their metabolites in human urine after cranberry-syrup consumption, *Food and Chemical Toxicology*. 55 (2013) 484–492. <https://doi.org/10.1016/j.fct.2013.01.039>.
- [33] N. Brindani, P. Mena, L. Calani, I. Benzie, S.-W. Choi, F. Brighenti, F. Zanardi, C. Curti, D. Del Rio, Synthetic and analytical strategies for the quantification of phenyl-γ-valerolactone conjugated metabolites in human urine, *Mol. Nutr. Food Res.* 61 (2017) 1700077. <https://doi.org/10.1002/mnfr.201700077>.
- [34] A. Stalmach, C.A. Edwards, J.D. Wightman, A. Crozier, Colonic catabolism of dietary phenolic and polyphenolic compounds from Concord grape juice, *Food Function*. 4 (2013) 52–62. <https://doi.org/10.1039/C2FO30151B>.
- [35] C. Li, X. Meng, B. Winnik, M.-J. Lee, H. Lu, S. Sheng, B. Buckley, C.S. Yang, Analysis of Urinary Metabolites of Tea Catechins by Liquid Chromatography/Electrospray Ionization Mass Spectrometry, *Chem. Res. Toxicol.* 14 (2001) 702–707. <https://doi.org/10.1021/tx0002536>.
- [36] K. Banaszewski, E. Park, I. Edirisinghe, J.C. Cappozzo, B.M. Burton-Freeman, A pilot study to investigate bioavailability of strawberry anthocyanins and characterize postprandial plasma polyphenols absorption patterns by Q-TOF LC/MS in humans, *Journal of Berry Research*. 3 (2013) 113–126. <https://doi.org/10.3233/JBR-130048>.
- [37] X. Zeng, W. Su, Y. Bai, T. Chen, Z. Yan, J. Wang, M. Su, Y. Zheng, W. Peng, H. Yao, Urinary metabolite profiling of flavonoids in Chinese volunteers after consumption of orange juice by UFLC-Q-TOF-MS/MS, *Journal of Chromatography B*. 1061–1062 (2017) 79–88. <https://doi.org/10.1016/j.jchromb.2017.07.015>.
- [38] R.P. Feliciano, E. Mecha, M.R. Bronze, A. Rodriguez-Mateos, Development and validation of a high-throughput micro solid-phase extraction method coupled with ultra-high-performance liquid chromatography-quadrupole time-of-flight mass spectrometry for rapid identification and quantification of phenolic metabolites in human plasma and urine, *Journal of Chromatography A*. 1464 (2016) 21–31. <https://doi.org/10.1016/j.chroma.2016.08.027>.

- [39] A.K. Sandhu, Y. Huang, D. Xiao, E. Park, I. Edirisinghe, B. Burton-Freeman, Pharmacokinetic Characterization and Bioavailability of Strawberry Anthocyanins Relative to Meal Intake, *J. Agric. Food Chem.* 64 (2016) 4891–4899. <https://doi.org/10.1021/acs.jafc.6b00805>.
- [40] A.K. Sandhu, M.G. Miller, N. Thangthaeng, T.M. Scott, B. Shukitt-Hale, I. Edirisinghe, B. Burton-Freeman, Metabolic fate of strawberry polyphenols after chronic intake in healthy older adults, *Food Funct.* 9 (2018) 96–106. <https://doi.org/10.1039/C7FO01843F>.
- [41] E. Mecha, R.P. Feliciano, A. Rodriguez-Mateos, S.D. Silva, M.E. Figueira, M.C. Vaz Patto, M.R. Bronze, Human bioavailability of phenolic compounds found in common beans: the use of high-resolution MS to evaluate inter-individual variability, *Br J Nutr.* 123 (2020) 273–292. <https://doi.org/10.1017/S0007114519002836>.
- [42] G. Pereira-Caro, J.L. Ordóñez, I. Ludwig, S. Gaillet, P. Mena, D. Del Rio, J.-M. Rouanet, K.A. Bindon, J.M. Moreno-Rojas, A. Crozier, Development and validation of an UHPLC-HRMS protocol for the analysis of flavan-3-ol metabolites and catabolites in urine, plasma and feces of rats fed a red wine proanthocyanidin extract, *Food Chemistry.* 252 (2018) 49–60. <https://doi.org/10.1016/j.foodchem.2018.01.083>.
- [43] M. Martínez-Huélamo, S. Tulipani, X. Torrado, R. Estruch, R.M. Lamuela-Raventós, Validation of a New LC-MS/MS Method for the Detection and Quantification of Phenolic Metabolites from Tomato Sauce in Biological Samples, *J. Agric. Food Chem.* 60 (2012) 4542–4549. <https://doi.org/10.1021/jf205266h>.
- [44] M. Wu, X. Wu, D. Zhang, F. Qiu, L. Ding, H. Ma, X. Chen, Metabolic profiling of quercetin in rats using ultra-performance liquid chromatography/quadrupole-time-of-flight mass spectrometry, *Biomedical Chromatography.* 31 (2017) e4016. <https://doi.org/10.1002/bmc.4016>.
- [45] J. Lee, S.E. Ebeler, J.A. Zweigenbaum, A.E. Mitchell, UHPLC-(ESI)QTOF MS/MS Profiling of Quercetin Metabolites in Human Plasma Postconsumption of Applesauce Enriched with Apple Peel and Onion, *J. Agric. Food Chem.* 60 (2012) 8510–8520. <https://doi.org/10.1021/jf302637t>.
- [46] M. Gómez-Juaristi, S. Martínez-López, B. Sarria, L. Bravo, R. Mateos, Absorption and metabolism of yerba mate phenolic compounds in humans, *Food Chemistry.* 240 (2018) 1028–1038. <https://doi.org/10.1016/j.foodchem.2017.08.003>.
- [47] N. Hayasaka, N. Shimizu, T. Komoda, S. Mohri, T. Tsushida, T. Eitsuka, T. Miyazawa, K. Nakagawa, Absorption and Metabolism of Luteolin in Rats and Humans in Relation to in Vitro Anti-inflammatory Effects, *J. Agric. Food Chem.* 66 (2018) 11320–11329. <https://doi.org/10.1021/acs.jafc.8b03273>.
- [48] W. Zhao, Z. Shang, Q. Li, M. Huang, W. He, Z. Wang, J. Zhang, Rapid Screening and Identification of Daidzein Metabolites in Rats Based on UHPLC-LTQ-Orbitrap Mass Spectrometry Coupled with Data-Mining Technologies, *Molecules.* 23 (2018) 151. <https://doi.org/10.3390/molecules23010151>.
- [49] S. Saha, P.A. Kroon, A Simple and Rapid LC-MS/MS Method for Quantification of Total Daidzein, Genistein, and Equol in Human Urine, *Journal of Analytical Methods in Chemistry.* 2020 (2020) 1–9. <https://doi.org/10.1155/2020/2359397>.
- [50] J. Zhang, Q. Guo, M. Wei, J. Bai, J. Huang, Y. Liu, Z. Su, X. Qiu, Metabolite Identification and Pharmacokinetic Profiling of Isoflavones from Black Soybean in Rats Using Ultrahigh-Performance Liquid Chromatography with Linear-Ion-Trap–Orbitrap and Triple-Quadrupole Tandem Mass Spectrometry, *J. Agric. Food Chem.* 66 (2018) 12941–12952. <https://doi.org/10.1021/acs.jafc.8b04852>.
- [51] S. Tulipani, M. Martinez Huelamo, M. Rotches Ribalta, R. Estruch, E.E. Ferrer, C. Andres-Lacueva, M. Illan, R.M. Lamuela-Raventós, Oil matrix effects on plasma exposure and urinary excretion of phenolic compounds from tomato sauces: Evidence from a human pilot study, *Food Chemistry.* 130 (2012) 581–590. <https://doi.org/10.1016/j.foodchem.2011.07.078>.

- [52] F. Castello, M.-S. Fernández-Pachón, I. Cerrillo, B. Escudero-López, Á. Ortega, A. Rosi, L. Bresciani, D. Del Rio, P. Mena, Absorption, metabolism, and excretion of orange juice (poly)phenols in humans: The effect of a controlled alcoholic fermentation, *Archives of Biochemistry and Biophysics*. 695 (2020) 108627. <https://doi.org/10.1016/j.abb.2020.108627>.
- [53] Q. Jiao, L. Xu, L. Jiang, Y. Jiang, J. Zhang, B. Liu, Metabolism study of hesperetin and hesperidin in rats by UHPLC-LTQ-Orbitrap MS ⁿ, *Xenobiotica*. 50 (2020) 1311–1322. <https://doi.org/10.1080/00498254.2019.1567956>.
- [54] C.D. Kay, G. Mazza, B.J. Holub, J. Wang, Anthocyanin metabolites in human urine and serum, *Br J Nutr*. 91 (2004) 933–942. <https://doi.org/10.1079/BJN20041126>.
- [55] I.A. Ludwig, P. Mena, L. Calani, G. Borges, G. Pereira-Caro, L. Bresciani, D. Del Rio, M.E.J. Lean, A. Crozier, New insights into the bioavailability of red raspberry anthocyanins and ellagitannins, *Free Radical Biology and Medicine*. 89 (2015) 758–769. <https://doi.org/10.1016/j.freeradbiomed.2015.10.400>.
- [56] D.N. Cooke, S. Thomasset, D.J. Boocock, M. Schwarz, P. Winterhalter, W.P. Steward, A.J. Gescher, T.H. Marczylo, Development of Analyses by High-Performance Liquid Chromatography and Liquid Chromatography/Tandem Mass Spectrometry of Bilberry (*Vaccinium myrtillus*) Anthocyanins in Human Plasma and Urine, *J. Agric. Food Chem*. 54 (2006) 7009–7013. <https://doi.org/10.1021/jf061562q>.
- [57] S. Yuste, A. Macià, I.A. Ludwig, M.-P. Romero, S. Fernández-Castillejo, Ú. Catalán, M.-J. Motilva, L. Rubió, Validation of Dried Blood Spot Cards to Determine Apple Phenolic Metabolites in Human Blood and Plasma After an Acute Intake of Red-Fleshed Apple Snack, *Mol. Nutr. Food Res*. 62 (2018) 1800623. <https://doi.org/10.1002/mnfr.201800623>.
- [58] M. Gómez-Juaristi, S. Martínez-López, B. Sarria, L. Bravo, R. Mateos, Bioavailability of hydroxycinnamates in an instant green/roasted coffee blend in humans. Identification of novel colonic metabolites, *Food Funct*. 9 (2018) 331–343. <https://doi.org/10.1039/C7FO01553D>.
- [59] J.K. Aschoff, K.M. Riedl, J.L. Cooperstone, J. Högel, A. Bosy-Westphal, S.J. Schwartz, R. Carle, R.M. Schweiggert, Urinary excretion of Citrus flavanones and their major catabolites after consumption of fresh oranges and pasteurized orange juice: A randomized cross-over study, *Mol. Nutr. Food Res*. 60 (2016) 2602–2610. <https://doi.org/10.1002/mnfr.201600315>.
- [60] C. Marmet, L. Actis-Goretta, M. Renouf, F. Giuffrida, Quantification of phenolic acids and their methylates, glucuronides, sulfates and lactones metabolites in human plasma by LC–MS/MS after oral ingestion of soluble coffee, *Journal of Pharmaceutical and Biomedical Analysis*. 88 (2014) 617–625. <https://doi.org/10.1016/j.jpba.2013.10.009>.
- [61] M. Martínez-Huélamó, A. Vallverdú-Queralt, G. Di Lecce, P. Valderas-Martínez, S. Tulipani, O. Jáuregui, E. Escribano-Ferrer, R. Estruch, M. Illan, R.M. Lamuela-Raventós, Bioavailability of tomato polyphenols is enhanced by processing and fat addition: Evidence from a randomized feeding trial, *Mol. Nutr. Food Res*. 60 (2016) 1578–1589. <https://doi.org/10.1002/mnfr.201500820>.
- [62] D. Scherbl, M. Renouf, C. Marmet, L. Poquet, I. Cristiani, S. Dahbane, S. Emady-Azar, J. Sauser, J. Galan, F. Dionisi, E. Richling, Breakfast consumption induces retarded release of chlorogenic acid metabolites in humans, *Eur Food Res Technol*. 243 (2017) 791–806. <https://doi.org/10.1007/s00217-016-2793-y>.
- [63] A. Esteban-Fernández, C. Ibañez, C. Simó, B. Bartolomé, M.V. Moreno-Arribas, An Ultrahigh-Performance Liquid Chromatography–Time-of-Flight Mass Spectrometry Metabolomic Approach to Studying the Impact of Moderate Red-Wine Consumption on Urinary Metabolome, *Journal of Proteome Research*. 17 (2018) 1624–1635.
- [64] Z. Zhang, M. Xu, S. Sun, X. Qiao, B. Wang, J. Han, D. Guo, Metabolic analysis of four phenolic acids in rat by liquid chromatography–tandem mass spectrometry, *J. Chromatogr. B*. 87 (2008) 7–14. <https://doi.org/10.1016/j.jchromb.2008.06.019>.

- [65] A. Stalmach, W. Mullen, D. Barron, K. Uchida, T. Yokota, C. Cavin, H. Steiling, G. Williamson, A. Crozier, Metabolite Profiling of Hydroxycinnamate Derivatives in Plasma and Urine after the Ingestion of Coffee by Humans: Identification of Biomarkers of Coffee Consumption, *Drug Metab Dispos.* 37 (2009) 1749–1758.
<https://doi.org/10.1124/dmd.109.028019>.
- [66] G. Pereira-Caro, M.N. Clifford, T. Polyviou, I.A. Ludwig, H. Alfheaid, J.M. Moreno-Rojas, A.L. Garcia, D. Malkova, A. Crozier, Plasma pharmacokinetics of (poly)phenol metabolites and catabolites after ingestion of orange juice by endurance trained men, *Free Radical Biology and Medicine.* 160 (2020) 784–795.
<https://doi.org/10.1016/j.freeradbiomed.2020.09.007>.
- [67] C. Favari, P. Mena, C. Curti, G. Istas, C. Heiss, D. Del Rio, A. Rodriguez-Mateos, Kinetic profile and urinary excretion of phenyl- γ -valerolactones upon consumption of cranberry: a dose–response relationship, *Food Funct.* 11 (2020) 3975–3985.
<https://doi.org/10.1039/D0FO00806K>.
- [68] A. Anesi, P. Mena, A. Bub, M. Ulaszewska, D. Del Rio, S.E. Kulling, F. Mattivi, Quantification of Urinary Phenyl- γ -Valerolactones and Related Valeric Acids in Human Urine on Consumption of Apples, *Metabolites.* 9 (2019) 254.
<https://doi.org/10.3390/metabo9110254>.
- [69] M. Rotches-Ribalta, C. Andres-Lacueva, R. Estruch, E. Escribano, M. Urpi-Sarda, Pharmacokinetics of resveratrol metabolic profile in healthy humans after moderate consumption of red wine and grape extract tablets, *Pharmacological Research.* 66 (2012) 375–382. <https://doi.org/10.1016/j.phrs.2012.08.001>.
- [70] Z. Qiu, J. Yu, Y. Dai, X. Chen, F. Huang, N. Li, A simple LC–MS/MS method for the simultaneous quantification of resveratrol and its major phase II metabolites: Assessment of their urinary and biliary excretions in rats, *Journal of Chromatography B.* 1048 (2017) 85–93. <https://doi.org/10.1016/j.jchromb.2017.02.011>.
- [71] L. Svila, J.-C. Martin, C. Defoort, C. Paut, F. Tourniaire, A. Brochot, Quantification of trans-resveratrol and its metabolites in human plasma using ultra-high performance liquid chromatography tandem quadrupole-orbitrap mass spectrometry, *Journal of Chromatography B.* 1104 (2019) 119–129. <https://doi.org/10.1016/j.jchromb.2018.11.016>.
- [72] C.A. Daykin, J.P.M.V. Duynhoven, A. Groenewegen, M. Dachtler, J.M.M.V. Amelsvoort, T.P.J. Mulder, Nuclear Magnetic Resonance Spectroscopic Based Studies of the Metabolism of Black Tea Polyphenols in Humans, *J. Agric. Food Chem.* 53 (2005) 1428–1434. <https://doi.org/10.1021/jf048439o>.