Food & Function

ROYAL SOCIETY OF CHEMISTRY

PAPER

View Article Online
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Cite this: *Food Funct.*, 2025, **16**, 3963

Extended recommendations on the nomenclature for microbial catabolites of dietary (poly)phenols, with a focus on isomers†

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There is an increasing body of evidence indicating that phenolic compounds derived from microbiota-mediated breakdown of dietary (poly)phenolics in the colon are at least partially responsible for the beneficial effects of a plant-based diet. Investigating the role of these catabolites and defining their particular biological effects is challenging due to the complex microbial pathways and the diversity of structures that are produced. When reviewing the data this is further exacerbated by the inconsistency and lack of standardization in naming the microbial phenolics. Here we update the nomenclature of colonic catabolites of dietary (poly)phenols, extending the proposals of Kay *et al.* (*Am. J. Clin. Nutr.*, 2020, **112**, 1051–1068, DOI: 10.1093/ajcn/nqaa204), by providing additional structures, and addressing the difficulties that can arise when investigating regioisomers and stereoisomers, where subtle differences in structure can have a substantial impact on bioactivity. The information provided will help to better harmonize the literature, facilitate data retrieval and provide a reference for researchers in several fields, especially nutrition and biochemistry.

Received 11th December 2024,
Accepted 12th February 2025

DOI: 10.1039/d4fo06152g

rsc.li/food-function

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† Electronic supplementary information (ESI) available. See DOI: https://doi.org/10.1039/D4FO06152G

1. Introduction

Growing attention is being focussed on the involvement of dietary (poly)phenols, including flavan-3-ols, anthocyanins and caffeoylquinic acids, in the protective effects of diets rich in fruits and vegetables on the development of a number of non-communicable chronic conditions including coronary heart disease, inflammation, diabetes, and reduced cognitive function.[1–6] Following ingestion, a portion of these compounds, many of which have a C_6–C_3–C_6 structure, are absorbed in the small intestine and appear in the circulation as phase-II glucuronide, methoxy and sulfate metabolites.[7] However, substantial amounts of the parent compounds pass to the lower bowel where they are broken down by the resident microbiota yielding a complex array of phenolic catabolites,[8] a number of which have been shown to exhibit properties in model systems related to anti-inflammatory, anti-adhesive, anti-estrogenic and angiotensin-converting enzyme inhibitory activities, as well as a reduction of neural cell oxidative damage, prevention of cancer and improvement of markers of gut barrier integrity.[9–23]

Investigations of the catabolism of dietary (poly)phenols in the lower gastrointestinal tract and the elucidation of protective effects of the resultant phenolic catabolites, and their use as biomarkers to modulate human health,[24–28] are compounded by the sheer number of catabolites involved, not just in biofluids but also plants and derived foods. This is further complicated by the variety of nomenclatures and trivial names used to describe the phenolic compounds involved.

In October 2020 a consortium of researchers published proposals for a convenient and unambiguous nomenclature for dietary (poly)phenol catabolites.[29] The current paper is an extension of this publication providing an expanded list of phenolics, accompanied by figures illustrating the listed structures. It is the natural consequence of testing the proposed standardized nomenclature and addresses some of the difficulties arising when naming catabolites that were not included in the first version. It also sheds light on the potential problems arising when dealing with regioisomers and stereoisomers. Isomers are known to differ in absorption, metabolism, pharmacokinetics and associated biological effects and these differences are an important topic that is frequently overlooked. The nomenclature of glutathione derivatives, which are produced in the upper GI tract, and the microbial catabolites of lignans, the so-called enterolignans, are also reviewed. This paper will serve as a new guideline for harmonized research approaches in the field of dietary (poly)phenols. The main groups of phenolics that are included are outlined in ESI.†

2. Nomenclature

Table 1 was established based on cross-referencing the following databases: PubChem (**https://pubchem.ncbi.nlm.nih.gov**), NIST Chemistry WebBook (**https://webbook.nist.gov/**), ChemIDPlus (**https://chem.nlm.nih.gov/chemidplus**), HMDB (**https://www.hmdb.ca**), ChemSpider (**https://www.chemspider.com**), ChemicalBook (**https://www.chemicalbook.com**), and ChEMBL (**https://www.ebi.ac.uk**) and follows the format adopted in the 2020 recommendations.[28] The recommended nomenclature is presented in column 1. The hyphenation of the compound names in this column has been standardized. However, whatever nomenclature system has been used in publications, the hyphenation can vary for many reasons, including typesetting, house style, lack of space in table columns, line breaks, *etc*., and is beyond the control of the authors. As a result, when searching for specific compounds in databases such as Web of Science or PubChem, it is essential to use "wildcards" or more than one system of hyphenation in the search term to locate as many occurrences as possible of the compound of interest. In future, it would be extremely helpful if search engines were designed to accommodate such variations in hyphenation.

Column 2 in Table 1 lists examples in bold of alternative "non-prime" nomenclature, followed by common synonyms, and often reported inaccurate nomenclature in italicized square brackets which should be avoided to prevent further confusion in the literature and in on-line databases.

When dealing with compounds such as 2,3-dihydroxybenzene-1-sulfate, a phase-II metabolite of 1,2,3-trihydroxybenzene (aka pyrogallol), for convenience, rather than using the full nomenclature throughout the text, it is acceptable to use the synonym pyrogallol-1-sulfate provided the recommended nomenclature is used on its first occurrence in the article. All glucuronic acid conjugations are β-D-configured and, as only oxygen-linked glucuronides have been detected, it is not necessary to include the *O*-linkage in the recommended name, *i.e.*, 3-(phenyl)propanoic acid-4′-glucuronide is sufficient. However, some journal editors/reviewers insist that the *O*-linkage is specified and, because it is not an incorrect notation it can, if necessary, be used.

Column 3 in Table 1 quotes the Chemical Abstracts Service (CAS) Registry Number which is a numeric identifier that can contain up to 10 digits, divided by hyphens into three parts. Each number is intended to be a unique numeric identifier that can link to information about the substance it refers to but has no chemical significance *per se* (**https://www.cas.org/support/documentation/chemical-substances/**). In principle, all compounds should have a distinct number, but some do not, presumably because they have a limited occurrence and/or no commercial source. Some compounds appear to have two numbers for reasons which are unclear.

In principle, each isomer should have a distinct number, with an additional number for a racemic mixture or a preparation where the constituent isomer(s) has not been determined, as illustrated in Table 1 with CAS numbers for 5-(3′,4′-dihydroxyphenyl)-γ-valerolactone (21618-92-8 (racemic), 1108192-01-3 (4*S*) and 191666-22-5 (4*R*)). This is also the case for geometric isomers, for example *trans*-cinnamic acid (140-10-3) and *cis*-cinnamic acid (102-94-3), where CAS 621-82-9 is used when geometry is not specified. However, 501-16-6 and 331-39-5 are both associated with *trans*-3′,4′-dihydroxycinnamic acid (aka caffeic acid), and "racemic 2-hydroxy-2-(4′-hydroxy-3′-methoxyphenyl)acetic acid" is associated with 2394-20-9 and 55-10-7.

Table 1 Recommendations for standardizing nomenclature for dietary (poly)phenol catabolites. Structures of the listed compounds are illustrated in (Fig. 1–10)

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
1. Hydroxybenzenes (C_6–C_0)			
1,2-Dihydroxybenzene [1.1]	Benzene-1,2-diol Catechol Pyrocatechol Brenzcatechin	120-80-9	Benzene-1,2-diol (YCIMNLLNPGFGHC-UHFFFAOYSA-N; 110.036779 g mol^{-1})
1,3-Dihydroxybenzene [1.2]	Benzene-1,3-diol Resorcinol	108-46-3	Benzene-1,3-diol (GHMLBKRAJCXXBS-UHFFFAOYSA-N; 110.036779 g mol^{-1})
1,2,3-Trihydroxybenzene [1.3]	Benzene-1,2,3-triol Pyrogallol	87-66-1	Benzene-1,2,3-triol (WQGWDDDVZFFDIG-UHFFFAOYSA-N; 126.031694 g mol^{-1})
1,3,5-Trihydroxybenzene [1.4]	Benzene-1,3,5-triol Phloroglucinol	108-73-6	Benzene-1,3,5-triol (QCDYQQDYXPDABM-UHFFFAOYSA-N; 126.031694 g mol^{-1})
4-Methyl-1,2-dihydroxybenzene [1.5]	4-Methyl-1,2-benzenediol 4-Methylcatechol *[3,4-Dihydroxytoluene]*	452-86-8	4-Methylbenzene-1,2-diol (ZBCATMYQYDCTIZ-UHFFFAOYSA-N; 124.052429 g mol^{-1})
2-Hydroxybenzene-1-sulfate [1.6]	*[Catechol-2-sulfate pyrocatechol sulfate]*	4918-96-1	(2-Hydroxyphenyl) hydrogen sulfate (MZPWKJZDOCIALD-UHFFFAOYSA-N; 189.993594 g mol^{-1})
2-Hydroxybenzene-1-glucuronide [1.7]	*[catechol-2-glucuronide catechol-glucuronide]*	28623-57-6	(2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-Trihydroxy-6-(2-hydroxyphenoxy)oxane-2-carboxylic acid (ICPYZFZFSLTYID-GOVZDWNOSA-N; 286.068867 g mol^{-1})
2,3-Dihydroxybenzene-1-sulfate [1.8]	*[pyrogallol-3-sulfate pyrogallol-1-sulfate]*	—	(2,3-Dihydroxyphenyl) hydrogen sulfate (NGVLEQPKHLWZLN-UHFFFAOYSA-N; 205.988509 g mol^{-1})
2,3-Dihydroxybenzene-1-glucuronide [1.9]	*[pyrogallol-3-glucuronide pyrogallol-1-glucuronide]*	—	— (302.066378 g mol^{-1})
2-Hydroxybenzene-1-glucuronide-3-sulfate [1.10]	*[pyrogallol-2-sulfate-3-glucuronide]*	—	— (382.02060 g mol^{-1})
2. Benzaldehydes (C_6–C_1)			
4-Hydroxybenzaldehyde [2.1]	4-Formylphenol	123-08-0	4-Hydroxybenzaldehyde (RGHHSNMVTDWUBI-UHFFFAOYSA-N; 122.036779 g mol^{-1})
3,4-Dihydroxybenzaldehyde [2.2]	Protocatechualdehyde	139-85-5	3,4-Dihydroxybenzaldehyde (IBGBGRVKPALMCQ-UHFFFAOYSA-N; 138.031694 g mol^{-1})
2,4,6-Trihydroxybenzaldehyde [2.3]	Phloroglucinaldehyde	487-70-7	2,4,6-Trihydroxybenzaldehyde (BTQAJGSMXCDDAJ-UHFFFAOYSA-N; 154.026609 g mol^{-1})
3-Hydroxy-4-methoxybenzaldehyde [2.4]	Isovanillin	621-59-0	3-Hydroxy-4-methoxybenzaldehyde (JVTZFYYHCGSXJV-UHFFFAOYSA-N; 152.047344 g mol^{-1})
4-Hydroxy-3-methoxybenzaldehyde [2.5]	3-Methoxy-4-hydroxybenzaldehyde Vanillin	121-33-5	4-Hydroxy-3-methoxybenzaldehyde (MWOOGOJBHIARFG-UHFFFAOYSA-N; 152.047344 g mol^{-1})
3. Benzoic acids (C_6–C_1)			
3-Hydroxybenzoic acid [3.1]	3-Hydroxybenzene carboxylic acid	99-06-9	3-Hydroxybenzoic acid (IJFXRHURBJZNAO-UHFFFAOYSA-N; 138.031694 g mol^{-1})
4-Hydroxybenzoic acid [3.2]	4-Hydroxybenzene carboxylic acid	99-96-7	4-Hydroxybenzoic acid (FJKROLUGYXJWQN-UHFFFAOYSA-N; 138.031694 g mol^{-1})
2,5-Dihydroxybenzoic acid [3.3]	Gentisic acid 5-Hydroxy-salicylic acid hydroquinone carboxylic acid	490-79-9	2,5-Dihydroxybenzoic acid (WXTMDXOMEHJXQO-UHFFFAOYSA-N; 154.026611 g mol^{-1})
3,4-Dihydroxybenzoic acid [3.4]	protocatechuic acid	99-50-3	3,4-Dihydroxybenzoic acid (YQUVCSBJEUQKSH-UHFFFAOYSA-N; 154.026609 g mol^{-1})
3,5-Dihydroxybenzoic acid [3.5]	α-Resorcylic acid	99-10-5	3,5-Dihydroxybenzoic acid (UYEMGAFJOZZIFP-UHFFFAOYSA-N; 154.026609 g mol^{-1})
3,4,5-Trihydroxybenzoic acid [3.6]	Gallic acid	149-91-7	3,4,5-Trihydroxybenzoic acid (LNTHITQWFMADLM-UHFFFAOYSA-N; 170.021523 g mol^{-1})
5-Hydroxy-2-aminobenzoic acid [3.7]	5-Hydroxyanthranilic acid	394-31-0	2-Amino-5-hydroxybenzoic acid

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
			(HYNQTSZBTIOFKH-UHFFFAOYSA-N; 153.042593 g mol^{-1})
Benzoic acid-4-glucuronide [3.8]	—	—	6-(4-Carboxyphenoxy)-3,4,5-trihydroxyoxane-2- carboxylic acid (DKNOHNCMCYDVLT-UHFFFAOYSA-N; 314.063782 g mol^{-1})
Benzoic acid-4-sulfate [3.9]	*[4-Hydroxybenzoic acid-4-O-sulphate]*	3233-38-3	4-(Sulfooxy)benzoic acid (RJTYSXVYCZAUHE-UHFFFAOYSA-N; 217.988509 g mol^{-1})
3-Hydroxybenzoic acid-4-glucuronide [3.10]	*[Protocatechuic acid-4-glucuronide]*	—	6-(4-Carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid (NLCBCVGRBFNEJE-UHFFFAOYSA-N; 330.058697 g mol^{-1})
4-Hydroxybenzoic acid-3-glucuronide [3.11]	*[protocatechuic acid-3-glucuronide]*	953037-17-7	6-(5-Carboxy-2-hydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid (CXNFDJSOAJNKSU-UHFFFAOYSA-N; 330.058697 g mol^{-1})
3-Hydroxybenzoic acid-4-sulfate [3.12]	*[protocatechuic acid-4-sulfate]*	38339-04-7	2-[3-Hydroxy-4-(sulfooxy)phenyl]acetic acid (ZQTJTTSZJNFQGJ-UHFFFAOYSA-N; 233.983423 g mol^{-1})
4-Hydroxybenzoic acid-3-sulfate [3.13]	*[Protocatechuic acid-3-sulfate]*	76496-11-2	4-Hydroxy-3-(sulfooxy)benzoic acid (GSFKEOSQCKWCLH-UHFFFAOYSA-N; 233.983423 g mol^{-1})
3-Hydroxy-4-methoxybenzoic acid [3.14]	Isovanillic acid	645-08-9	3-Hydroxy-4-methoxybenzoic acid (LBKFGYZQBSGRHY-UHFFFAOYSA-N; 168.042259 g mol^{-1})
4-Methoxybenzoic acid-3-glucuronide[3.15]	*[Isovanillic acid-3-glucuronide]*	—	6-(5-Carboxy-2-methoxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid (WREVRVHLTSYMIJ-UHFFFAOYSA-N; 344.074347 g mol^{-1})
4-Methoxybenzoic acid-3-sulfate [3.16]	*[isovanillic acid-3-sulfate]*	—	4-methoxy-3-(sulfooxy)benzoic acid (VSFFJSSUGMYRMP-UHFFFAOYSA-N; 247.999073 g mol^{-1})
4-Hydroxy-3-methoxybenzoic acid [3.17]	Vanillic acid	121-34-6	4-hydroxy-3-methoxybenzoic acid (WKOLLVMJNQIZCI-UHFFFAOYSA-N; 168.042259 g mol^{-1})
3-Methoxybenzoic acid-4-glucuronide [3.18]	*[Vanillic acid-4-glucuronide]*	—	(2*S*,3*S*,4*R*,5*R*,6*S*)-6-(4-Carboxy-2-methoxyphenoxy)-3,4-dihydroxy-5-methyloxane-2-carboxylic acid (MBNPZIKKKDDLLL-QGZCQISNSA-N; 344.074347 g mol^{-1})
3-Methoxybenzoic acid-4-sulfate[3.19]	*[Vanillic acid-4-sulfate]*	71235-86-4	3-Methoxy-4-sulfooxybenzoic acid (TXRKUXPAEPOCIX-UHFFFAOYSA-N; 247.999073 g mol^{-1})
4-Hydroxy-3,5-dimethoxybenzoic acid [3.20]	Syringic acid	530-57-4	4-Hydroxy-3,5-dimethoxybenzoic acid (JMSVCTWVEWCHDZ-UHFFFAOYSA-N; 198.052823 g mol^{-1})
3,4-Dimethoxybenzoic acid [3.21]	veratric acid	93-07-2	3,4-Dimethoxybenzoic acid (DAUAQNGYDSHRET-UHFFFAOYSA-N; 182.057909 g mol^{-1})
4. Cinnamic acids (C_6–C_3 unsaturated)[a]			
cinnamic acid [4.1]	*trans*-Cinnamic acid	621-82-9 140-10-3	(2*E*)-3-Phenylprop-2-enoic acid (WBYWAXJHAXSJNI-VOTSOKGWSA-N; 148.052429 g mol^{-1})
2′-Hydroxycinnamic acid [4.2]	**2-Hydroxycinnamic acid** *o*-Coumaric acid *trans*-2-Coumaric acid *trans*-2-Hydroxycinnamic acid 3-(2-Hydroxyphenyl)acrylic acid	614-60-8	(2*E*)-3-(2-Hydroxyphenyl)prop-2-enoic acid (PMOWTIHVNWZYFI-AATRIKPKSA-N; 164.047344 g mol^{-1})
3′-Hydroxycinnamic acid [4.3]	**3-Hydroxycinnamic acid** *m*-Coumaric acid 3-Coumaric acid *trans*-3-Coumaric acid 3-(3-Hydroxyphenyl)acrylic acid	588-30-7	(2*E*)-3-(3-Hydroxyphenyl)prop-2-enoic acid (KKSDGJDHHZEWEP-SNAWJCMRSA-N; 164.047344 g mol^{-1})
4′-Hydroxycinnamic acid [4.4]	**4-hydroxycinnamic acid** Coumaric acid *p*-Coumaric acid 4-Coumaric acid *trans*-4-Hydroxycinnamic acid 4-Hydroxyphenyl)acrylic acid	501-98-4	(2*E*)-3-(4-Hydroxyphenyl)prop-2-enoic acid (NGSWKAQJJWESNS-ZZXKWVIFSA-N; 164.047344 g mol^{-1})

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
3′,4′-Dihydroxycinnamic acid [4.5]	**3,4-Dihydroxycinnamic acid** Caffeic acid 501-16-6 *trans*-Caffeic acid 3-(3,4-Dihydroxyphenyl)acrylic acid	331-39-5	(2*E*)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid (QAIPRVGONGVQAS-DUXPYHPUSA-N; 180.042259 g mol^{-1})
Cinnamic acid-4′-glucuronide [4.6]	**Cinnamic acid-4-glucuronide** *[p-Coumaric acid-4′-glucuronide]*	—	(2*S*,3*S*,4*R*,5*R*,6*S*)-6-{4-[(1*E*)-2-Carboxyeth-1-en-1-yl]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid (SOKJXEKPKWKYKR-LZJCFMAWSA-N; 340.079432 g mol^{-1})
4′-Hydroxy-3′-methoxycinnamic acid [4.7]	**4-Hydroxy-3-methoxycinnamic acid** Ferulic acid 537-98-4 *trans*-Ferulic acid 3-(4-Hydroxy-3-methoxyphenyl)acrylic acid	537-98-4	(2*E*)-3-(4-Hydroxy-3-methoxyphenyl)prop-2-enoic acid (KSEBMYQBYZTDHS-HWKANZROSA-N; 194.057909 g mol^{-1})
3′-Methoxycinnamic acid-4′-glucuronide [4.8]	**3-Methoxycinnamic acid-4-glucuronide** *[Ferulic acid-4-glucuronide]*	86321-24-6	— 370.089996 g mol^{-1}
3′-Methoxycinnamic acid-4′-sulfate [4.9]	**3-Methoxycinnamic acid-4-sulfate** *[Ferulic acid-4′-sulfate* *Ferulic acid-4-sulfate]*	86321-29-1	(*E*)-3-(3-Methoxy-4-sulfooxyphenyl)prop-2-enoic acid (PZPATWACAAOHTJ-HWKANZROSA-N; 274.014723 g mol^{-1})
3′-Hydroxy-4′-methoxycinnamic acid [4.10]	**3-hydroxy-4-methoxycinnamic acid** Isoferulic acid 537-73-5 Hesperetate 3-(3-Hydroxy-4-methoxyphenyl)acrylic acid	537-73-5	(2*E*)-3-(3-Hydroxy-4-methoxyphenyl)prop-2-enoic acid (QURCVMIEKCOAJU-HWKANZROSA-N; 194.057909 g mol^{-1})
4′-Methoxycinnamic acid-3′-glucuronide [4.11]	**4-Methoxycinnamic acid-3-glucuronide** *[Isoferulic acid-3′-glucuronide* *Isoferulic acid-3-glucuronide]*	1065272-10-7	(2*S*,3*S*,4*S*,5*R*,6*S*)-6-[5-[(*E*)-2-carboxyethenyl]-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid (SHJZLGVIOYFHCB-MBAOVNHDSA-N; 370.089996 g mol^{-1})
4′-Methoxycinnamic acid-3′-sulfate [4.12]	**4-methoxycinnamic acid-3-sulfate** *[Isoferulic acid-3-sulfate* *Isoferulic acid-3-sulfate]*	1258842-19-1	(*E*)-3-(4-Methoxy-3-sulfooxyphenyl)prop-2-enoic acid (DCMKMHVTKFJMAU-HWKANZROSA-N; 274.014723 g mol^{-1})
5. Phenylpropanoic acids (C_6–C_3)			
3-Phenylpropanoic acid [5.1]	3-(Phenyl)propanoic acid *[Dihydrocinnamic acid* *Hydrocinnamic acid]*	501-52-0	3-Phenylpropanoic acid (XMIIGOLPHOKFCH-UHFFFAOYSA-N; 150.06808 g mol^{-1})
3-(3′-Hydroxyphenyl)propanoic acid [5.2]	**3-(3-Hydroxyphenyl)propanoic acid** 3-(3-Hydroxyphenyl)propionic acid 3-Hydroxy-dihydrocinnamic acid *m*-Hydroxy-dihydrocinnamic acid	621-54-5	3-(3-Hydroxyphenyl)propanoic acid (QVWAEZJXDYOKEH-UHFFFAOYSA-N; 166.062994 g mol^{-1})
3-(4′-Hydroxyphenyl)propanoic acid [5.3]	**3-(4-Hydroxyphenyl)propanoic acid** 3-(4-Hydroxyphenyl)propionic acid 4-Hydroxy-dihydrocinnamic acid *m*-Hydroxy-dihydrocinnamic acid *m*-Hydroxy-hydrocinnamic acid Phloretic acid	501-97-3	3-(4-Hydroxyphenyl)propanoic acid (NMHMNPHRMNGLLB-UHFFFAOYSA-N; 166.062994 g mol^{-1})
3-(3′,4′-Dihydroxyphenyl)propanoic acid [5.4]	**3-(3,4-Dihydroxyphenyl)propanoic acid** 3-(3,4-Dihydroxyphenyl)propionic acid Dihydrocaffeic acid Hydrocaffeic acid 3,4-Dihydroxybenzenepropanoic acid 3,4-Dihydroxy-dihydrocinnamic acid	1078-61-1	3-(3,4-Dihydroxyphenyl)propanoic acid (DZAUWHJDUNRCTF-UHFFFAOYSA-N; 182.057909 g mol^{-1})
3-(3′,5′-Dihydroxyphenyl)propanoic acid [5.5]	**3-(3,5-Dihydroxyphenyl)propanoic acid** 3-(3,5-Dihydroxyphenyl)propionic acid 3,5-Dihydroxybenzenepropanoic acid 3,5-Dihydroxy-dihydrocinnamic acid 3,5-Dihydroxy-hydrocinnamic acid	26539-01-5	3-(3,5-Dihydroxyphenyl)propanoic acid (ITPFIKQWNDGDLG-UHFFFAOYSA-N; 182.057909 g mol^{-1})

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
3-(Phenyl)propanoic acid-4′-glucuronide [**5.6**]	**3-(Phenyl)propanoic acid-4-glucuronide** 3-(Phenyl)propionic acid-4-glucuronide *[4-Hydroxy-dihydrocinnamic acid-4-glucuronide* *p-Hydroxy-dihydrocinnamic acid-glucuronide]*	—	— 342.095082 g mol^{-1}
3-(3′-Methoxyphenyl)propanoic acid [**5.7**]	**3-(3-Methoxyphenyl)propanoic acid** 3-(3-Methoxyphenyl)propionic acid 3-Methoxy-dihydrocinnamic acid	10516-71-9	3-(3-Methoxyphenyl)propanoic acid (BJJQJLOZWBZEGA-UHFFFAOYSA-N; 180.07864425 g mol^{-1})
3-(4′-Methoxyphenyl)propanoic acid [**5.8**]	**3-(4-Methoxyphenyl)propanoic acid** 3-(4-Methoxyphenyl)propionic acid 4-Methoxy-dihydrocinnamic acid	1929-29-9	3-(4-Methoxyphenyl)propanoic acid (FIUFLISGGHNPSM-UHFFFAOYSA-N; 180.078644 g mol^{-1})
3-(3′-Hydroxy-4′-methoxyphenyl)propanoic acid [**5.9**]	**3-(3-Hydroxy-4-methoxyphenyl)propanoic acid** Dihydro-isoferulic acid 3-(3-Hydroxy-4-methoxyphenyl)dihydrocinnamic acid	1135-15-5	3-(3-Hydroxy-4-methoxyphenyl)propanoic acid (ZVIJTQFTLXXGJA-UHFFFAOYSA-N; 196.073559 g mol^{-1})
3-(4′-Hydroxy-3′-methoxyphenyl)propanoic acid [**5.10**]	**3-(4-Hydroxy-3-methoxyphenyl)propanoic acid** 3-(4-Hydroxy-3-methoxyphenyl)propionic acid Dihydroferulic acid *[Hydroferulic acid]* 3-(4-Hydroxy-3-methoxyphenyl)dihydrocinnamic acid	1135-23-5	3-(4-hydroxy-3-methoxyphenyl) propanoic acid (BOLQJTPHPSDZHR-UHFFFAOYSA-N; 196.073559 g mol^{-1})
3-(4′-Hydroxyphenyl)propanoic acid-3′-glucuronide [**5.11**]	**3-(4-Hydroxyphenyl)propanoic acid-3-glucuronide** 3-(4-Hydroxyphenyl)propionic acid-3-glucuronide *[Dihydrocaffeic acid-3′-glucuronide* *Dihydrocaffeic acid-3-glucuronide]*	1187945-71-6	(2*S*,3*S*,4*S*,5*R*,6*S*)-6-[5-(2-Carboxyethyl)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid (AELQNMHOLDHBFA-DKBOKBLXSA-N; 358.089997 g mol^{-1})
3-(3′-Hydroxyphenyl)propanoic acid-4′-glucuronide [**5.11**]	**3-(3-Hydroxyphenyl)propanoic acid-4-glucuronide** 3-(3-Hydroxyphenyl)propionic acid-4-glucuronide *[Dihydrocaffeic acid-4′-glucuronide* *Dihydrocaffeic acid-4-glucuronide]*	—	(2*S*,3*S*,4*S*,5*R*)-6-[4-(2-CARBOXYETHYL)-2-hydroxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid (DUTJMLCURMYWCW-HXMBFPRCSA-N; 358.089997 g mol^{-1})
3-(3′-Hydroxyphenyl)propanoic acid-4′-sulfate [**5.13**]	**3-(3-Hydroxyphenyl)propanoic acid-4-sulfate** 3-(3-Hydroxyphenyl)propionic acid-4-sulfate *[Dihydrocaffeic acid-4′-sulfate* *Dihydrocaffeic acid-4-sulfate]*	—	3-(3-Hydroxy-4-sulfooxyphenyl)propanoic acid (WEPNMLSXEATIJK-UHFFFAOYSA-N; 262.014723 g mol^{-1})
3-(4′-Hydroxyphenyl)propanoic acid-3′-sulfate [**5.14**]	**3-(4-Hydroxyphenyl)propanoic acid-3-sulfate** 3-(4-Hydroxyphenyl)propionic acid-3-sulfate *[Dihydrocaffeic acid-3′-sulfate* *Dihydrocaffeic acid-3-sulfate]*	1187945-70-5	3-[4-Hydroxy-3-(sulfooxy)phenyl]propanoic acid (MIMULQQHBAZGER-UHFFFAOYSA-N; 262.014724 g mol^{-1})
3-(3′-Methoxyphenyl)propanoic acid-4′-glucuronide [**5.15**]	**3-(3-Methoxyphenyl)propanoic acid-4-glucuronide** 3-(3-Methoxyphenyl)propionic acid-4-glucuronide *[Dihydroferulic acid-4′-glucuronide* *Dihydroferulic acid-4-glucuronide]*	86321-28-0	(2*S*,3*S*,4*S*,5*R*,6*S*)-6-[4-(2-carboxyethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid (KYERCTIKYSSKPA-JHZZJYKESA-N; 372.105646 g mol^{-1})
3-(3′-Methoxyphenyl)propanoic acid-4′-sulfate [**5.16**]	**3-(3-Methoxyphenyl)propanoic acid-4-sulfate** 3-(3-Methoxyphenyl)propionic acid-4-sulfate *[Dihydroferulic acid-4′-sulfate* *Dihydroferulic acid-4-sulfate]*	86321-33-7	3-(3-Methoxy-4-sulfooxyphenyl)propanoic acid (UMCDODPBPQMWQP-UHFFFAOYSA-N; 276.030374 g mol^{-1})
3-(4′-Methoxyphenyl)propanoic acid-3′-glucuronide [**5.17**]	**3-(4-Methoxyphenyl)propanoic acid-3-glucuronide**	1187945-72-7	(2*S*,3*S*,4*S*,5*R*,6*S*)-6-[5-(2-Carboxyethyl)-2-methoxyphenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
	3-(4-Methoxyphenyl)propionic acid-3-Glucuronide *[Dihydro-isoferulic acid-3′-glucuronide]*		(SYLIYWIQUHQCPY-UHFFFAOYSA-N; 372.105647 g mol^{-1})
3-(4′-Methoxyphenyl)propanoic acid-3′-sulfate [5.18]	**3-(4-Methoxyphenyl)propanoic acid-3-sulfate** 3-(4-Methoxyphenyl)propionic acid-3-sulfate *[Dihydro-isoferulic acid-3′-sulfate* *Dihydro-isoferulic acid-3-sulfate]*	1258842-21-5	3-(4-Methoxy-3-sulfooxyphenyl)propanoic acid (QZIYZVFIROFZCV-UHFFFAOYSA-N; 276.030374 g mol^{-1})
6. Hydroxy-3-(phenyl)propanoic acids (C_6–C_3)			
(*R*/*S*)-3-Hydroxy-3-(phenyl)propanoic acid [6.1]	**3-(Phenyl)-3-hydroxypropanoic acid** 3-(Phenyl)hydracrylic acid	3480-87-3	3-Hydroxy-3-phenylpropanoic acid (AYOLELPCNDVZKZ-UHFFFAOYSA-N; 166.062994 g mol^{-1})
(*R*/*S*)-3-Hydroxy-3-(3′-hydroxyphenyl)propanoic acid [6.2]	**3-Hydroxy-3-(3-hydroxyphenyl)propanoic acid** 3-(3-Hydroxyphenyl)-3-hydroxypropionic acid 3-Hydroxy-3-(3′-hydroxyphenyl)propionic acid 3-Hydroxy-3-(3-hydroxyphenyl)propionic acid β, *m*-Dihydroxyphenylpropionic acid β, *meta*-dihydroxyphenylpropionic acid 3-(3-Hydroxyphenyl)hydracrylic acid 3-(3′-Hydroxyphenyl)hydracrylic acid *m*-Hydroxyphenylhydracrylic acid	3247-75-4	3-Hydroxy-3-(3-hydroxyphenyl)propanoic acid (KHTAGVZHYUZYMF-UHFFFAOYSA-N; 182.057909 g mol^{-1})
(*R*/*S*)-3-Hydroxy-3-(3′-hydroxy-4′-methoxyphenyl) propanoic acid [6.3]	**3-Hydroxy-3-(3-hydroxy-4-methoxyphenyl)propanoic acid** 3-Hydroxy-3-(3-hydroxy-4-methoxyphenyl)propionic acid 3-(3-Hydroxy-4-methoxyphenyl)-3-hydroxypropanoic acid 3-(3-Hydroxy-4-methoxyphenyl)-3-hydroxypropionic acid 3-(3′-Hydroxy-4′-methoxyphenyl)hydracrylic acid 3-(3-Hydroxy-4-methoxyphenyl)hydracrylic acid	28030-22-0	3-Hydroxy-3-(3-hydroxy-4-methoxyphenyl)propanoic acid (JEXBTMWMYGBBHO-UHFFFAOYSA-N; 212.068473 g mol^{-1})
(*R*/*S*)-2-Hydroxy-3-(phenyl)propanoic acid [6.4]	**3-(Phenyl)-2-hydroxypropanoic acid** 2-Hydroxy-3-(phenyl)propionic acid 3-(Phenyl)-2-hydroxypropionic acid 3-(Phenyl)lactic acid	828-01-3	2-Hydroxy-3-phenylpropionic acid; (VOXXWSYKYCBWHO-UHFFFAOYSA-N; 166.062994 g mol^{-1})
(*R*/*S*)-2-Hydroxy-3-(4′-hydroxyphenyl)propanoic acid [6.5]	**2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid** 3-(4-Hydroxyphenyl)-2-hydroxypropanoic acid 2-Hydroxy-3-(4-hydroxyphenyl)propionic acid 3-(4′-Hydroxyphenyl)-2-hydroxypropionic acid 3-(4′-Hydroxyphenyl)lactic acid 3-(4-Hydroxyphenyl)lactic acid	306-23-0	2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid (JVGVDSSUAVXRDY-UHFFFAOYSA-N; 182.057909 g mol^{-1})
(*R*/*S*)-2-Hydroxy-3-(3′,4′-dihydroxyphenyl)propanoic acid [6.6]	**2-Hydroxy-3-(3,4-dihydroxyphenyl)propanoic acid** 3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid 2-Hydroxy-3-(3′,4′-dihydroxyphenyl)propionic acid 3-(3,4-Dihydroxyphenyl)-2-hydroxypropionic acid 3-(3′,4′-Dihydroxyphenyl)lactic acid 3-(3,4-Dihydroxyphenyl)lactic acid Danshensu Salvianic acid	23028-17-3	3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid (PAFLSMZLRSPALU-UHFFFAOYSA-N; 198.052823 g mol^{-1})
7. Phenylacetic acids (C_6–C_2)			
phenylacetic acid [7.1]	Phenylethanoic acid 2-Phenylethanoate	103-82-2	2-Phenylacetic acid (WLJVXDMOQOGPHL-UHFFFAOYSA-N; 136.052429 g mol^{-1})

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
3′-Hydroxyphenylacetic Acid [7.2]	**3-Hydroxyphenylacetic acid** 3-Hydroxyphenylethanoic acid	621-37-4	2-(3-Hydroxyphenyl)acetic acid (FVMDYYGIDFPZAX-UHFFFAOYSA-N; 152.047344 g mol^{-1})
3′-Methoxyphenylacetic acid [7.3]	**3-Methoxyphenylacetic acid** 3-Methoxyphenylethanoic acid	1798-09-0	2-(3-Methoxyphenyl)acetic acid (LEGPZHPSIPPYIO-UHFFFAOYSA-N; 166.062994 g mol^{-1})
4′-Hydroxyphenylacetic acid [7.4]	**4-Hydroxyphenylacetic acid** 4-Hydroxyphenylethanoic acid	156-38-7	2-(4-Hydroxyphenyl)acetic acid (XQXPVVBIMDBYFF-UHFFFAOYSA-N; 152.047344 g mol^{-1})
3′,4′-Dihydroxyphenylacetic acid [7.5]	**3,4-Dihydroxyphenylacetic acid** 3,4-Dihydroxyphenylethanoic acid Homoprotocatechuic acid DOPAC	102-32-9	2-(3,4-Dihydroxyphenyl)acetic acid (CFFZDZCDUFSOFZ-UHFFFAOYSA-N; 168.042259 g mol^{-1})
4′-Hydroxy-3′-methoxyphenylacetic acid [7.6]	**4-Hydroxy-3-methoxyphenylacetic acid** 4-Hydroxy-3-methoxyphanylethanoic acid Homovanillic acid	306-08-1	2-(4-Hydroxy-3-methoxyphenyl)acetic acid (QRMZSPFSDQBLIX-UHFFFAOYSA-N; 182.057909 g mol^{-1})
8. Hydroxy-2-(phenyl)acetic acids (C_6–C_2)			
(*R*/*S*)-2-Hydroxy-2-(3′-hydroxyphenyl)acetic acid [8.1]	**2-Hydroxy-2-(3-hydroxyphenyl)acetic acid** (3-Hydroxyphenyl)-2-hydroxyacetic acid 2-Hydroxy-2-(3-hydroxyphenyl)ethanoic acid (3-Hydroxyphenyl)-2-hydroxyethanoic acid 3-Hydroxymandelic acid	17119-15-2	2-Hydroxy-2-(3-hydroxyphenyl)acetic acid (OLSDAJRAVOVKLG-UHFFFAOYSA-N; 168.042259 g mol^{-1})
(*R*/*S*)-2-Hydroxy-2-(4′-hydroxyphenyl)acetic acid [8.2]	**2-Hydroxy-2-(4-hydroxyphenyl)acetic acid** (4-Hydroxyphenyl)-2-hydroxyacetic acid 2-Hydroxy-2-(4′-hydroxyphenyl)ethanoic acid (4-Hydroxyphenyl)-2-hydroxyethanoic acid 4′-Hydroxymandelic acid 4-Hydroxymandelic acid 4-Hydroxy-D-mandelic acid 4-Hydroxy-L-mandelic acid	1198-84-1	2-Hydroxy-2-(4-hydroxyphenyl)acetic acid (YHXHKYRQLYQUIH-UHFFFAOYSA-N; 168.042259 g mol^{-1})
(*R*/*S*)-2-hydroxy-2-(4′-hydroxy-3′-methoxyphenyl) acetic acid [8.3]	**2-Hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid**	2394-20-9	2-Hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid
	(4-Hydroxy-3-methoxyphenyl)-2-hydroxyacetic acid 2-Hydroxy-2-(4-hydroxy-3-methoxyphenyl)ethanoic acid (4-Hydroxy-3-methoxyphenyl)-2-hydroxyethanoic acid 4′-Hydroxy-3′-methoxymandelic acid 4-Hydroxy-3-methoxymandelic acid 3-Methoxy-4-hydroxymandelic acid 4-Hydroxy-3-methoxy-L-mandelic acid Vanillylmandelic acid	55-10-7	(CGQCWMIAEPEHNQ-UHFFFAOYSA-N; 198.052823 g mol^{-1})
9. Hippuric acids (C_6–C_1–N<) and other amino acid conjugates			
hippuric acid [9.1]	—	495-69-2	2-Benzamidoacetic acid (QIAFMBKCNZACKA-UHFFFAOYSA-N; 179.058243 g mol^{-1})
2′-Hydroxyhippuric acid [9.2]	**2-Hydroxyhippuric acid** 2-(2-Hydroxybenzamido)acetic acid *N*-(2-Hydroxybenzoyl)glycine Salicyluric acid	487-54-7	2-[(2-Hydroxybenzoyl)amino]acetic acid (ONJSZLXSECQROL-UHFFFAOYSA-N; 195.053158 g mol^{-1})
3′-Hydroxyhippuric acid [9.3]	**3-Hydroxyhippuric acid** 2-(3-Hydroxybenzamido)acetic acid *N*-(3-Hydroxybenzoyl)glycine	1637-75-8	2-[(3-hydroxybenzoyl)amino]acetic acid (XDOFWFNMYJRHEW-UHFFFAOYSA-N; 195.053158 g mol^{-1})
4′-Hydroxyhippuric acid [9.4]	**4-Hydroxyhippuric acid** 2-(4-Hydroxybenzamido)acetic acid *N*-(4-Hydroxybenzoyl)glycine	2482-25-9	2-[(4-Hydroxybenzoyl)amino]acetic acid (ZMHLUFWWWPBTIU-UHFFFAOYSA-N; 195.053158 g mol^{-1})

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
4′-Methoxyhippuric acid [9.5]	**4-Methoxyhippuric acid** 2-(4-Ethoxybenzamido)acetic acid *N*-(4-Methoxybenzoyl)glycine	13214-64-7	2-[(4-Methoxybenzoyl)amino]acetic acid (SIEIOUWSTGWJGE-UHFFFAOYSA-N; 209.068808 g mol^{-1})
(*R*/*S*)-2-Hydroxyhippuric acid [9.6]	α-Hydroxyhippuric acid α-Hydroxybenzoylglycine *[2-hydroxyhipuric acid]*	16555-77-4	2-Hydroxy-2-(phenylformamido)acetic acid (GCWCVCCEIQXUQU-UHFFFAOYSA-N; 195.053158 g mol^{-1})
4′-Hydroxy-3′-methoxyhippuric acid [9.7]	4′-Hydroxy-3′-methoxybenzoyl-glycine vanilloyl-glycine	1212-04-0	2-[(4-Hydroxy-3-methoxybenzoyl)amino]acetic acid (LOODYTDRRBLQNH-UHFFFAOYSA-N; 225.063722 g mol^{-1})
3′-Hydroxy-4′-methoxyhippuric acid [9.8]	3′-Hydroxy-4′-methoxybenzoyl-glycine Isovanilloyl-glycine	22005-43-2	2-[(3-Hydroxy-4-methoxybenzoyl)amino]acetic acid (HOZJFFMWTLPBCS-UHFFFAOYSA-N; 225.063722 g mol^{-1})
Phenylacetyl-glycine [9.9]	Phenaceturic acid *[Phenylaceturic acid]*	500-98-1	2-[(2-Phenyacetyl)amino]acetic acid (UTYVDVLMYQPLQB-UHFFFAOYSA-N; 193.073893 g mol^{-1})
4′-Hydroxyphenylacetyl-glycine [9.10]	**4-Hydroxyphenylacetyl-glycine** 2-[-2-(4-Hydroxyphenyl)acetamido]acetic acid	28116-23-6	2-[[2-(4-Hydroxyphenyl)acetyl]amino]acetic acid (CPPDWYIPKSSNNM-UHFFFAOYSA-N; 209.068808 g mol^{-1})
(*S*)-Phenyacetyl-glutamine [9.11]	(2*S*)-5-Amino-5-oxo-2-(2-phenylacetamido)pentanoic acid Phenylacetyl-L-glutamine	28047-15-6	(2*S*)-5-Amino-5-oxo-2-(2-phenylacetamido)pentanoic acid (JFLIEFSWGNOPJJ-JTQLQIEISA-N; 264.111007 g mol^{-1})
(*S*)-4′-Hydroxyphenylacetyl-glutamine [9.12]	**4-Hydroxyphenylacetyl-glutamine** 2-[2-(4-Hydroxyphenyl)acetamido]pentanedioic acid	—	2-[[2-(4-Hydroxyphenyl)acetyl]amino]pentanedioic acid (CYRKYXZJUIBBJX-UHFFFAOYSA-N; 281.089937 g mol^{-1})
Cinnamoyl-glycine [9.13]	2-Cinnamamidoacetic acid	16534-24-0	2-[[(*E*)-3-Phenylprop-2-enoyl]amino]acetic acid (YAADMLWHGMUGQL-VOTSOKGWSA-N; 205.073893 g mol^{-1})
4′-Hydroxycinnamoyl-glycine [9.14]	**4-Hydroxycinnamoyl-glycine** *p*-coumaroyl-glycine	—	2-[[(*E*)-3-(4-Hydroxyphenyl)prop-2-enoyl]amino]acetic acid (NZSACLXQEHBCNF-ZZXKWVIFSA-N; 221.068807 g mol^{-1})
4′-Hydroxy-3′-methoxycinnamoyl-glycine [9.15]	**4-Hydroxy-3-methoxycinnamoyl-glycine** Feruloyl-glycine *N*-(3-Methoxycoumaroyl)-glycine 2-(3-Phenylpropanoylamino)acetic acid	1220-05-9	2-[[(*E*)-3-(4-Hydroxy-3-methoxyphenyl)prop-2-enoyl]amino]acetic acid (CLGNQAIRBLDHIN-HWKANZROSA-N; 251.079373 g mol^{-1})
3-(Phenyl)propanoyl-glycine [9.16]	*N*-(3-Phenylpropanoyl)glycine 2-(3-Phenylpropanoylamino)acetic acid	56613-60-6	2-(3-Phenylpropanoylamino)acetic acid (YEIQSAXUPKPPBN-UHFFFAOYSA-N; 207.089543 g mol^{-1})
10. Phenyl-γ-valerolactones (C_6–C_5)[b] (All compounds may occur as *R*- and *S*-enantiomers)			
(*R*/*S*)-5-(3′,4′-Dihydroxyphenyl)-γ-valerolactone [10.1]	**5-(3,4-Dihydroxyphenyl)-γ-valerolactone** δ-(3,4-Dihydroxyphenyl)-γ-valerolactone 5-(dihydroxyphenyl)-γ-valerolactone 5-(dihydroxyphenyl)-valerolactone *[M6]*	21618-92-8 1108192-01-3 (4*S*) 191666-22-5 (4*R*)	5-[(3,4-Dihydroxyphenyl)methyl]oxolan-2-one (ZNXXWTPQHVLMQT-UHFFFAOYSA-N; 208.073559 g mol^{-1})
(*R*/*S*)-5-(4′-Hydroxyphenyl)-γ-valerolactone-3′-glucuronide [10.2]	**5-(4-Hydroxyphenyl)-γ-valerolactone-3-glucuronide** *[M6-glucuronide 5-(3′,4′-dihydroxyphenyl)-γ-valerolactone-3′-glucuronide]*	—	3,4,5-Trihydroxy-6-[2-hydroxy-5-[(5-oxooxolan-2-yl)methyl]phenoxy]oxane-2-carboxylic acid (UVGDTVGPBRLMQY-UHFFFAOYSA-N; 384.105647 g mol^{-1})
(*R*/*S*)-5-(3′-Hydroxyphenyl)-γ-valerolactone-4′-glucuronide [10.3]	**5-(3-Hydroxyphenyl)-γ-valerolactone-4-glucuronide** *[M6-glucuronide-5-(3′,4′-dihydroxyphenyl)-γ-valerolactone-4′-glucuronide]*	—	3,4,5-Trihydroxy-6-{2-hydroxy-4-[(5-oxooxolan-2-yl)methyl]phenoxy}oxane-2-carboxylic acid (OTBJYBQGMPICIK-UHFFFAOYSA-N; 384.105647 g mol^{-1})
(*R*/*S*)-5-(4′-Hydroxyphenyl)-γ-valerolactone-3′-sulfate [10.4]	**5-(4-Hydroxyphenyl)-γ-valerolactone-3-sulfate**	—	[2-Hydroxy-5-[(5-oxooxolan-2-yl)methyl]phenyl] hydrogen sulfate

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
	[M6-sulfate 5-(3′,4′-dihydroxyphenyl)-γ-valerolactone-3′-sulfate]		(YAXFVDUJDAQPTJ-UHFFFAOYSA-N; 288.030374 g mol^{-1})
(*R*/*S*)-5-(3′-Hydroxyphenyl)-γ-valerolactone-4′-sulfate [10.5]	**5-(3-Hydroxyphenyl)-γ-valerolactone-4-sulfate**	—	[2-Hydroxy-4-[(5-oxooxolan-2-yl)methyl]phenyl] hydrogen sulfate
	[M6-sulfate 5-(3′4′-dihydroxyphenyl)-γ-valerolactone-4′-sulfate]		(WAXYAOJFDCCESK-UHFFFAOYSA-N; 288.030374 g mol^{-1})
(*R*/*S*)-5-(3′-Methoxyphenyl)-γ-valerolactone-4′-glucuronide [10.6]	**5-(3-Methoxyphenyl)-γ-valerolactone-4-glucuronide**	—	3,4,5-Trihydroxy-6-[2-methoxy-4-[(5-oxooxolan-2-yl)methyl] phenoxy]oxane-2-carboxylic acid
	[methyl-M6-glucuronide 5-(4′-hydroxy-3′-methoxyphenyl)-γ-valerolactone-4′-glucuronide 5-(3′,4′-dihydroxyphenyl)-γ-valerolactone-3′-methoxy-4′-glucuronide]		(NGMVEYPQYAIGEI-UHFFFAOYSA-N; 398.121297 g mol^{-1})
(*R*/*S*)-5-(3′-Methoxyphenyl)-γ-valerolactone-4′-sulfate [10.7]	**5-(3-Methoxyphenyl)-γ-valerolactone-4-sulfate**	—	[2-Methoxy-4-[(5-oxooxolan-2-yl)methyl]phenyl] hydrogen sulfate
	[methyl-M6-sulfate 5-(4′-hydroxy-3′-methoxyphenyl)-γ-valerolactone-4′-sulfate 5-(3′,4′-dihydroxyphenyl)-γ-valerolactone-3′-methoxy-4′-sulfate]		(FYRRHCSCZYSADR-UHFFFAOYSA-N; 302.046024 g mol^{-1})
(*R*/*S*)-5-(4′-Methoxyphenyl)-γ-valerolactone-3′-glucuronide [10.8]	**5-(4-Methoxyphenyl)-γ-valerolactone-3-glucuronide**	—	—
	[5-(3′,4′-Dihdroxyphenyl)-γ-valerolactone-4′-methoxy-3′-glucuronide]		398.121297 g mol^{-1}
(*R*/*S*)-5-(Phenyl)-γ-valerolactone-3′-sulfate-4′-glucuronide [10.9]	**5-(Phenyl)-γ-valerolactone-3-sulfate-4-glucuronide**	—	—
	[M6-sulfate-glucuronide 5-(3′,4′-dihydroxyphenyl)-γ-valerolactone-3′-sulfate-4′-glucuronide]		464.062461 g mol^{-1}
11. 4-Hydroxy-5-(phenyl)valeric acids (All compounds may occur as *R*- and *S*-enantiomers)			
(*R*/*S*)-4-hydroxy-5-(3′,4′-dihydroxyphenyl)valeric acid [11.1]	**4-Hydroxy-5-(3,4-dihydroxyphenyl)valeric acid**	—	5-(3,4-Dihydroxyphenyl)-4-hydroxypentanoic acid
	5-(3,4-Dihydroxyphenyl)-4-hydroxyvaleric acid 4-Hydroxy-5-(3,4-dihydroxyphenyl)pentanoic acid 5-(3,4-Dihydroxyphenyl)-4-hydroxypentanoic acid *[5-(3,4-Dihydroxyphenyl)-γ-hydroxyvaleric acid 5-(3,4-dihydroxyphenyl)-γ-hydroxypentanoic acid]*		(JDBYFCLHVYVXCX-UHFFFAOYSA-N; 226.084124 g mol^{-1})
(*R*/*S*)-4-Hydroxy-5-(4′-hydroxyphenyl)valeric acid-3′-glucuronide [11.2]	**4-Hydroxy-5-(4-hydroxyphenyl)valeric acid-3-glucuronide**	—	6-[5-(4-Carboxy-2-hydroxybutyl)-2-hydroxyphenoxy]-
	5-(4-hydroxyphenyl)-4-hydroxyvaleric acid-3-glucuronide 4-hydroxy-5-(4-hydroxyphenyl)pentanoic acid-3-glucuronide 5-(4-hydroxyphenyl)-4-hydroxypentanoic acid-3-glucuronide *[5-(3,4-dihydroxyphenyl-4-hydroxyvaleric acid-3-glucuronide]*		3,4,5-Trihydroxyoxane-2-carboxylic acid (BKJQCPDRWDNBIN-UHFFFAOYSA-N; 402.116212 g mol^{-1})
(*R*/*S*)-4-Hydroxy-5-(3′-hydroxyphenyl)valeric acid-4′-glucuronide [11.3]	**4-Hydroxy-5-(3-hydroxyphenyl)valeric acid-4-glucuronide**	—	6-[4-(4-Carboxy-2-hydroxybutyl)-2-hydroxyphenoxy]-
	5-(3-Hydroxyphenyl)-4-hydroxyvaleric acid-4-glucuronide		3,4,5-Trihydroxyoxane-2-carboxylic acid

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
	4-Hydroxy-5-(3-hydroxyphenyl)pentanoic acid-4-glucuronide 5-(4-Hydroxyphenyl)-4-hydroxyvaleric acid-4-glucuronide *[5-(3′,4′-Dihydroxyphenyl)-4-hydroxyvaleric acid-4′-glucuronide]*		(LLKUARGHNZMSRT-UHFFFAOYSA-N; 402.116212 g mol^{-1})
(*R*/*S*)-4-Hydroxy-5-(4′-hydroxyphenyl)valeric acid-3′-sulfate [11.4]	**4-Hydroxy-5-(4-hydroxyphenyl)valeric acid-3-sulfate**	—	4-Hydroxy-5-(4-hydroxy-3-sulfooxyphenyl)pentanoic acid
	5-(4-Hydroxyphenyl)-4-hydroxyvaleric acid-3-sulfate 4-Hydroxy-5-(4-hydroxyphenyl)pentanoic acid-3-sulfate 5-(4-Hydroxyphenyl)-4-hydroxypentanoic acid-3-sulfate *[5-(3′,4′-Dihydroxyphenyl)-4-hydroxyvaleric acid-3′-sulfate]*		(HROSNTXKMPHTSL-UHFFFAOYSA-N; 306.040939 g mol^{-1})
(*R*/*S*)-4-Hydroxy-5-(3′-hydroxyphenyl)valeric acid-4′-sulfate [11.5]	**4-Hydroxy-5-(3-hydroxyphenyl)valeric acid-4-sulfate**	—	—
	5-(3-Hydroxyphenyl)-4-hydroxyvaleric acid-4-sulfate 4-Hydroxy-5-(3-hydroxyphenyl)pentanoic acid-4-sulfate 5-(3-Hydroxyphenyl)-4-hydroxypentanoic acid-4-sulfate *[5-(3′,4′-Dihydroxyphenyl)-4-hydroxyvaleric acid-4′-sulfate]*		306.040938 g mol^{-1}
(*R*/*S*)-4-Hydroxy-5-(3′-methoxyphenyl)valeric acid-4′-glucuronide [11.6]	**4-Hydroxy-5-(3-methoxyphenyl)valeric acid-4-glucuronide**	—	6-[4-(4-Carboxy-2-hydroxybutyl)-2-methoxyphenoxy]-3,4,5-Trihydroxyoxane-2-carboxylic acid
	5-(3-Methoxyphenyl)-4-hydroxyvaleric acid-4-glucuronide 4-Hydroxy-5-(3-methoxyphenyl)pentanoic acid-4-glucuronide 5-(3′-Methoxyphenyl)-4-hydroxypentanoic acid-4-glucuronide *[4-Hydroxy-5-(3′,4′-dihydroxyphenyl)-valeric acid-3′-methoxy-4′-glucuronide]*		(WOBDOUCWWPCYBL-UHFFFAOYSA-N; 416.131862 g mol^{-1})
(*R*/*S*)-4-Hydroxy-5-(3′-methoxyphenyl)valeric acid-4′-sulfate [11.7]	**4-Hydroxy-5-(3-methoxyphenyl)valeric acid-4-sulfate**	—	4-Hydroxy-5-[3-methoxy-4-(sulfooxy)phenyl]pentanoic acid
	5-(3-Methoxyphenyl)-4-hydroxyvaleric acid-4-sulfate 4-Hydroxy-5-(3-methoxyphenyl)pentanoic acid-4-sulfate 5-(3-Methoxyphenyl)-4-hydroxypentanoic acid-4-sulfate *[4-Hydroxy-5-(3,4-dihydroxyphenyl)-valeric acid-3-methoxy-4-sulfate]*		(GUEAZORXKKSCMA-UHFFFAOYSA-N; 320.056589 g mol^{-1})
(*R*/*S*)-4-Hydroxy-5-(4′-methoxyphenyl)valeric acid-3′-sulfate [11.8]	**4-Hydroxy-5-(4-methoxyphenyl)valeric acid-3-sulfate**	—	—

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
	5-(4-Methoxyphenyl)-4-hydroxyvaleric acid-3-sulfate 4-Hydroxy-5-(4′-methoxyphenyl)pentanoic acid-3′-sulfate 5-(4-Methoxyphenyl)-4-hydroxpentanoic acid-3-sulfate *[4-hydroxy-5-(3,4-dihydroxyphenyl)-valeric acid-3-methoxy-4-sulfate]*		(MFHSGCMDDUKYSZ-UHFFFAOYSA-N; 320.056589 g mol^{-1})
(*R*/*S*)-5-(3′,4′-Dihydroxyphenyl)valeric acid-4-sulfate [**11.9**]	**4-Sulfoxy-5-(3,4-dihydroxyphenyl)valeric acid** 5-(3,4-Dihydroxyphenyl)-4-sulfoxyvaleric acid 4-Sulfoxy-5-(3,4-dihydroxyphenyl)pentanoic acid 5-(3,4-Dihydroxyphenyl)-4-sulfoxypentanoic acid *[5-(3-Hydroxyphenyl)-4-sulphoxyvaleric acid]*	—	5-(3,4-Dihydroxyphenyl)-4-sulfooxypentanoic acid (NBKHZVHBUVNGQF-UHFFFAOYSA-N; 306.040939 g mol^{-1})
(*R*/*S*)-5-(4′-Hydroxy-3′-methoxyphenyl)valeric acid-4-sulfate [**11.10**]	**4-Sulfoxy-5-(4-hydroxy-3-methoxyphenyl)valeric acid** 5-(4-Hydroxy-3-methoxyphenyl)-4-sulfoxyvaleric acid 4-Sulfoxy-5-(4-hydroxy-3-methoxyphenyl)pentanoic acid 5-(4-Hydroxy-3-methoxyphenyl)-4-sulfoxypentanoic acid *[4-Hydroxy-5-(3,4-dihydroxyphenyl)-valeric acid-3-methoxy-4-sulfate]*	–	5-(4-Hydroxy-3-methoxyphenyl)-4-(sulfooxy)pentanoic acid (JQISKEAFUDWLCF-UHFFFAOYSA-N; 320.056589 g mol^{-1})
12. 5-Phenylvaleric acids (C_6–C_5)			
5-(3′,5′-Dihydroxyphenyl)valeric acid [**12.1**]	**5-(3,5-Dihydroxyphenyl)valeric acid** 5-(3,5-Dihydroxyphenyl)pentanoic acid *[5-(Dihydroxyphenyl)valeric acid]*	74356-41-5	5-(3,5-Dihydroxyphenyl)pentanoic acid (QHXNJIMVPAFCPR-UHFFFAOYSA-N; 210.089203 g mol^{-1})
5-(3′,4′,5′-Trihydroxyphenyl)valeric acid [**12.2**]	**5-(3,4,5-Trihydroxyphenyl)valeric acid** 5-(3,4,5-Trihydroxyphenyl)pentanoic acid *[5-(Trihydroxyphenyl)valeric acid]*	—	5-(3,4,5-Trihydroxyphenyl)pentanoic acid (MASHJJSDLKLZLA-UHFFFAOYSA-N; 226.084124 g mol^{-1})
13. Urolithins (6*H*-dibenzo[*b*,*d*]pyran-6-ones)			
3-Hydroxy-urolithin [**13.1**]	urolithin B	1139-83-9	3-Hydroxy-6*H*-benzo[*c*]chromen-6-one (WXUQMTRHPNOXBV-UHFFFAOYSA-N; 212.047344 g mol^{-1})
Urolithin-3-glucuronide [**13.2**]	Urolithin B-3-glucuronide *[Urolithin B-glucuronide]*	823806-74-2	(2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-trihydroxy-6-({6-oxo-6*H*-benzo[*c*]chromen-3-yl}oxy)oxane-2-carboxylic acid (MHBWCULXQBVPQT-KSPMYQCISA-N; 388.079432 g mol^{-1})
Urolithin-3-sulfate [**13.3**]	Urolithin B-3-sulfate *[Urolithin B-sulfate]*	—	6-Oxobenzo[*c*]chromen-3-yl) hydrogen sulfate (LRRVKQQFGIEMSA-UHFFFAOYSA-N; 292.004159 g mol^{-1})
3,8-Dihydroxy-urolithin [**13.4**]	Urolithin A	1143-70-0	3,8-Dihydroxy-6*H*-benzo[*c*]chromen-6-one (RIUPLDUFZCXCHM-UHFFFAOYSA-N; 228.042259 g mol^{-1})
3,9-Dihydroxy-urolithin [**13.5**]	Isourolithin A	174023-48-4	3,9-Dihydroxy-6*H*-benzo[*c*]chromen-6-one (WDGSXHQNUPZEHA-UHFFFAOYSA-N; 228.042259 g mol^{-1})
8-Hydroxy-urolithin-3-glucuronide [**13.6**]	Urolithin A-3-glucuronide *[urolithin A-glucuronide 3,8-dihydroxy-urolithin 3-glucuronide]*	—	3,4,5-Trihydroxy-6-(8-hydroxy-6-oxo-6*H*-benzo[*c*]chromen-3-yl) oxyoxane-2-carboxylic acid (KXBXNRJGUDTJQS-UHFFFAOYSA-N; 404.074347 g mol^{-1})
3-Hydroxy-urolithin-8-glucuronide [**13.7**]	urolithin A-8-glucuronide	1365982-52-0	(2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-trihydroxy-6-(3-hydroxy-6-oxobenzo[*c*]chromen-8-yl)oxyoxane-2-carboxylic acid

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
	[Urolithin A-glucuronide 3,8-dihydroxy-urolithin 8-glucuronide]		(QMPHAAMUHRNZSL-KSPMYQCISA-N; 404.074347 g mol^{-1})
8-Hydroxy-urolithin-3-sulfate [13.8]	Urolithin A-3-sulfate *[Urolithin A-sulfate 3,8-dihydroxy-urolithin 3-sulfate]*	—	(8-Hydroxy-6-oxobenzo[*c*]chromen-3-yl) hydrogen sulfate (WMPNAWQWWZFJTQ-UHFFFAOYSA-N; 307.999074 g mol^{-1})
3-Hydroxy-urolithin-8-sulfate [13.9]	Urolithin A-8-sulfate *[Urolithin A-sulfate 3,8-dihydroxy-urolithin 8-sulfate]*	—	(3-Hydroxy-6-oxo-6*H*-benzo[*c*]chromen-8-yl)oxidanesulfonic acid (307.999074 g mol^{-1})
9-Hydroxy-urolithin-3-glucuronide [13.10]	Isourolithin A-3-glucuronide *[Isourolithin A-glucuronide 3,9-dihydroxy-urolithin-3-glucuronide]*	—	— 404.074347 g mol^{-1}
3-Hydroxy-urolithin-9-glucuronide [13.11]	isourolithin A-9-glucuronide *[Isourolithin A-glucuronide, 3,9-dihydroxy-urolithin 9-glucuronide]*	1268248-75-4	— 404.074347 g mol^{-1}
Urolithin-3,8-diglucuronide [13.12]	Urolithin A-3,8-diglucuronide *[Urolithin A-diglucuronide 3,8-dihydroxy-urolithin-diglucuronide]*	—	(2*S*,3*S*,4*S*,5*R*,6*S*)-6-[3-[(2*S*,3*R*,4*S*,5*S*,6*S*)-6-carboxy-3,4,5-trihydroxyoxan-2-yl]oxy-6-oxobenzo[*c*]chromen-8-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid (SXMJSEFKPOZNAT-ILJCXFEASA-N; 580.106435 g mol^{-1})
Urolithin-3-sulfate-8-glucuronide [13.13]	*[Urolithin A-sulfate-glucuronide 3,8-dihydroxy-urolithin 3-sulfate-8-glucuronide]*	—	— 484.03116 g mol^{-1}
3,8,9-Trihydroxy-urolithin [13.14]	Urolithin C *[Hydroxyurolithin A trihydroxyurolithin]*	165393-06-6	3,8,9-Trihydroxy-6*H*-benzo[*c*]chromen-6-one (HHXMEXZVPJFAIJ-UHFFFAOYSA-N; 244.037173 g mol^{-1})
3,8,10-Trihydroxy-urolithin [13.15]	Urolithin M7	531512-26-2	3,8,10-Trihydroxy-6*H*-benzo[*c*]chromen-6-one (AKJHSPSPAOUDFT-UHFFFAOYSA-N; 244.037173 g mol^{-1})
8,9-Dihydroxy-urolithin-3-glucuronide [13.16]	Urolithin C-3-glucuronide *[urolithin C-glucuronide]*	1268248-76-5	(2*S*,3*S*,4*S*,5*R*,6*S*)-6-({8,9-Dihydroxy-6-oxo-6*H*-benzo[*c*]chromen-3-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid (DDAQYQCCOWZGDO-KSPMYQCISA-N; 420.069261 g mol^{-1})
3,4,8,9-Tetrahydroxy-urolithin [13.17]	Urolithin D	131086-98-1	3,4,8,9-Tetrahydroxy-6*H*-benzo[*c*]chromen-6-one (NEZDQSKPNPRYAW-UHFFFAOYSA-N; 260.032088 g mol^{-1})
3,8,9,10-Tetrahydroxy-urolithin [13.18]	Urolithin M6	1006683-97-1	3,8,9,10-Tetrahydroxy-6*H*-benzo[*c*]chromen-6-one (LGXFTZDSEIQMMP-UHFFFAOYSA-N; 260.032088 g mol^{-1})
14. Stilbenoids[a]			
dihydroresveratrol [14.1]	Dihydro-resveratrol 5-(4-Hydroxyphenethyl)benzene-1,3-diol 3,4′,5-Trihydroxybibenzyl Dihydro-3,4′,5-trihydroxystilbene	58436-28-5	5-[2-(4-Hydroxyphenyl)ethyl]benzene-1,3-diol (HITJFUSPLYBJPE-UHFFFAOYSA-N; 230.094294 g mol^{-1})
lunularin [14.2]	3-(4-Hydroxyphenethyl)phenol 3,4′-Dihydroxydihydrostilbene 3,4′-Ethylenebisphenol 3,4′-Dihydroxybibenzyl	37116-80-6	3-[2-(4-Hydroxyphenyl)ethyl]phenol (ILEYXPCRQKRNIJ-UHFFFAOYSA-N; 214.099380 g mol^{-1})
3,4′-Dihydroxy-*trans*-stilbene [14.3]	3,4′-Dihydroxystilbene Stilbene-3,4′-diol	62574-04-3	3-[2-(4-Hydroxyphenyl)ethenyl]phenol (UFGKEFGYNRJIGO-UHFFFAOYSA-N; 212.083730 g mol^{-1})
4-Hydroxydibenzyl [14.4]	4-Phenylethylphenol *p*-Phenylethylphenol	6335-83-7	4-(2-Phenylethyl)phenol (YTLSTADDHMJUMW-UHFFFAOYSA-N; 198.104465 g mol^{-1})
15. Anthranilic acid (2-aminobenzoic acid) derivatives			
Dihydroavenanthramide D [15.1]	2-[[3-(4-Hydroxyphenyl)-1-oxopropyl]amino]benzoic acid 2-(3-(4-Hydroxyphenyl)propanamido)benzoic acid Hydroxyphenyl propamidobenzoic acid	697235-49-7	2-[3-(4-Hydroxyphenyl)propanoylamino]benzoic acid (DLFOKZQWYFNKCL-UHFFFAOYSA-N; 285.100108 g mol^{-1})
2-Acetamido-5-hydroxybenzoic acid [15.2]	2-(Acetylamino)-5-hydroxybenzoic acid	1882-76-4	2-Acetamido-5-hydroxybenzoic acid

Table 1 *(Contd.)*

Recommended names	Non-prime names, synonyms and incorrect nomenclature *[italics]*	CAS	IUPAC (InChIKey; Monoisotopic Mass Da.)
			(DXKBECZFNWKIJC-UHFFFAOYSA-N; 195.053157 g mol^{-1})
5-Hydroxy-2-aminobenzoic acid [15.3]	2-Amino-5-hydroxybenzoic acid 5-Hydroxyanthranilic acid	394-31-0	2-Amino-5-hydroxybenzoic acid (HYNQTSZBTIOFKH-UHFFFAOYSA-N; 153.042593 g mol^{-1})
16. Phenylethanols (C_6–C_2)			
2-(4′-Hydroxyphenyl)ethanol [16.1]	**2-(4-Hydroxyphenyl)ethanol** 4-Hydroxyphenyl alcohol 4-Hydroxyphenethyl alcohol Tyrosol *p*-HPEA	501-94-0	4-(2-Hydroxyethyl)phenol (YCCILVSKPBXVIP-UHFFFAOYSA-N; 138.06808 g mol^{-1})
2-(3′-4′-Dihydroxyphenyl)ethanol [16.2]	**2-(3,4-Hydroxyphenyl)ethanol** 3′-Hydroxytyrosol 3,4-Dihydroxyphenylethanol 3,4-Dihydroxyphenethyl alcohol DOPET Homoprotocatechuyl alcohol	10597-60-1	4-(2-Hydroxyethyl)-1,2-benzenediol (JUUBCHWRXWPFFH-UHFFFAOYSA-N; 154.062994 g mol^{-1})
2-(Phenyl)ethanol-4′-glucuronide [16.3]	**2-(Phenyl)ethanol-4-glucuronide** Tyrosol-4-glucuronide Tyrosol-4′-glucuronide	28116-28-1	(2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-Trihydroxy-6-[4-(2-hydroxyethyl)phenoxy] oxane-2-carboxylic acid (HEIHXCBRTPYOMU-BYNIDDHOSA-N; 314.100167 g mol^{-1})
2-(Phenyl)ethanol-4′-sulfate [16.4]	**2-(Phenyl)ethanol-4-sulfate** Tyrosol-4-sulfate Tyrosol-4′-sulfate	—	[4-(2-Hydroxyethyl)phenyl] hydrogen sulfate (VCRXMIQBQGCAAL-UHFFFAOYSA-N; 218.024895 g mol^{-1})
2-(4′-Hydroxyphenyl)ethanol-3′-glucuronide [16.5]	**2-(4-Hydroxyphenyl)ethanol-3-glucuronide** Hydroxytyrosol-3-glucuronide Hydroxytyrosol-3′-glucuronide	425408-50-0	(2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-Trihydroxy-6-[2-hydroxy-5-(2-hydroxyethyl)phenoxy]oxane-2-carboxylic acid (CPHMFZSEPDNJAZ-BYNIDDHOSA-N; 330.095082 g mol^{-1})
2-(3′-Hydroxyphenyl)ethanol-4′-glucuronide [16.6]	**2-(3-Hydroxyphenyl)ethanol-4-glucuronide** Hydroxytyrosol-4-glucuronide Hydroxytyrosol-4′-glucuronide	—	(2*S*,3*S*,4*S*,5*R*,6*S*)-3,4,5-Trihydroxy-6-[2-hydroxy-4-(2-hydroxyethyl)phenoxy]oxane-2-carboxylic acid (JMDNSUMWVYKARS-BYNIDDHOSA-N; 330.095082 g mol^{-1})
2-(4′-Hydroxyphenyl)ethanol-3′-sulfate [16.7]	**2-(4-Hydroxyphenyl)ethanol-3-sulfate** Hydroxytyrosol-3-sulfate Hydroxytyrosol-3′-sulfate	844639-92-5	[2-hydroXy-5-(2-hydroxyethyl)phenyl] hydrogen sulfate (BZTHVCCNFBAISK-UHFFFAOYSA-N; 234.019809 g mol^{-1})
2-(3′-Hydroxyphenyl)ethanol-4′-sulfate [16.8]	**2-(3-Hydroxyphenyl)ethanol-4-sulfate** Hydroxytyrosol-4-sulfate Hydroxytyrosol-4′-sulfate	425408-51-1	[2-Hydroxy-4-(2-hydroxyethyl)phenyl] hydrogen sulfate (VNPXBLBTQUFCHO-UHFFFAOYSA-N; 234.019809 g mol^{-1})

[a] Cinnamic acids and stilbenes have *cis* (*Z*) and *trans* (*E*) geometric isomers. In nature the *trans* isomer is more common. [b] In rare instances compounds appear to have two different InChIKey formulas in online databases which are generally associated with different CAS or registry numbers and possibly reflect uncharacterized isomeric configuration. For example: 5-(3′,4′-dihydroxyphenyl)-γ-valerolactone or IUPAC 5-[(3,4-dihydroxyphenyl)methyl]oxolan-2-one is listed as having two different CAS/RN, 21618-92-8 and 191666-22-5, two different standard 27 character InchIKey ZNXXWTPQHVLMQT-UHFFFAOYSA-N and ZNXXWTPQHVLMQT-MRVPVSSYSA-N and sharing the same SMILES formula C1CC(=O)OC1CC2=CC(=C(C=C2)O)O. In this case each structure has a unique Full InChIKey (using the SHA-256 algorithm) InChI = 1*S*/C11H12O4/c12-9-3-1-7(6-10(9)13)5-8-2-4-11(14)15-8/h1,3,6,8,12-13*H*,2,4-5H2, and 1*S*/C11H12O4/c12-9-3-1-7(6-10(9)13)5-8-2-4-11(14)15-8/h1,3,6,8,12-13*H*,2,4-5H2/t8-/m1/s1, which should be used in cases where two isomers require distinction. Similarly, 5-(3′-hydroxyphenyl)-γ-valerolactone-4′-glucuronide or IUPAC 3,4,5-trihydroxy-6-{2-hydroxy-4-[(5-oxooxolan-2-yl)methyl]phenoxy}oxane-2-carboxylic acid, has two different standard InChIKey: OTBJYBQGMPICIK-UHFFFAOYSA -N and OTBJYBQGMPICIK-GHPVWUPISA-N, and different SMILES formula and full InChIKey.

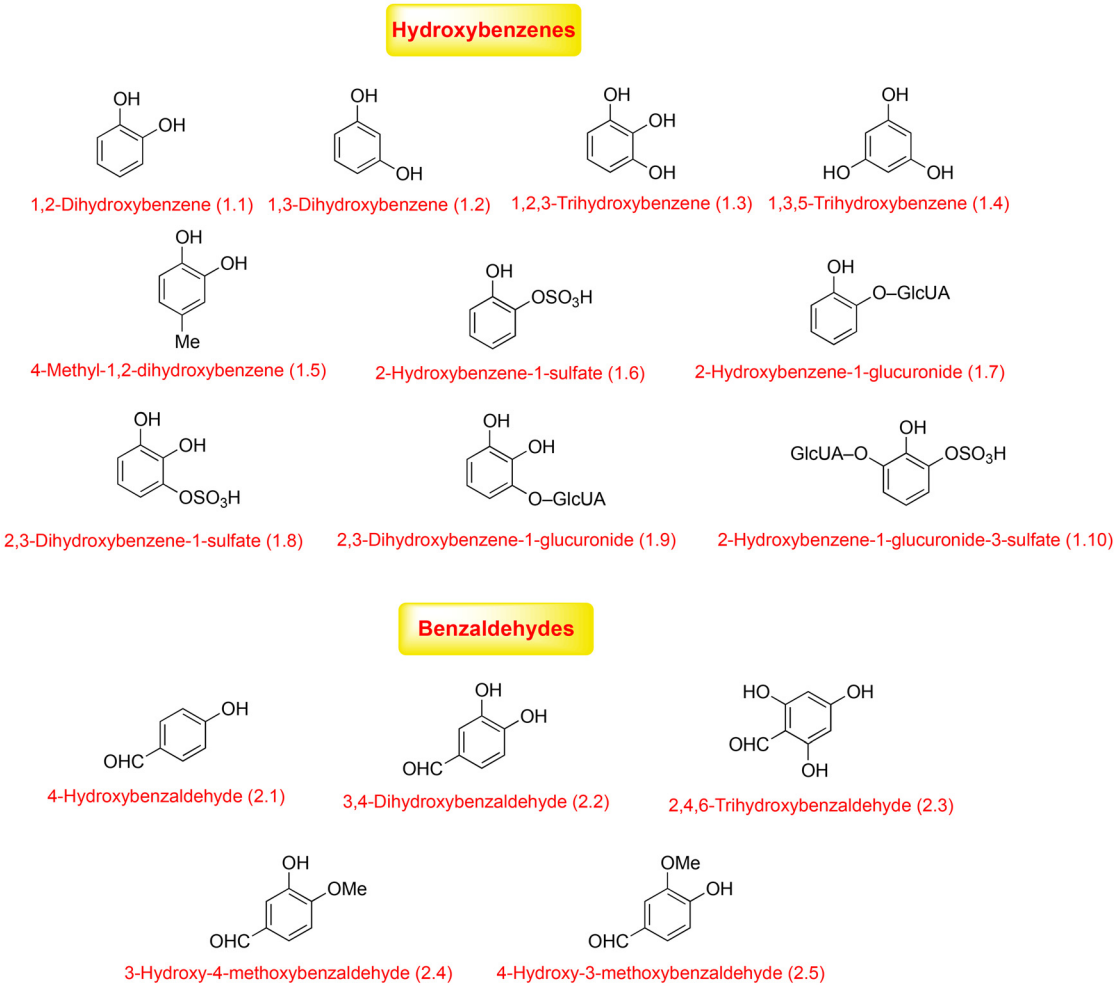

Fig. 1 Structures of hydroxybenzenes (**1.1–1.10**) and benzaldehydes (**2.1–2.5**). GlcUA – β-D-glucuronide.

The International Union of Pure and Applied Chemistry (IUPAC) is described as the world authority on chemical nomenclature and terminology (**https://iupac.org/who-we-are/**). This nomenclature is found in column 4 together with the InChIKey, which is the IUPAC standard textual unique chemical identifier, along with the isotopic mass in daltons (Table 1).

New compounds in Table 1 since Kay *et al.*[29] include the resveratrol catabolites dihydroresveratrol (**14.1**), lunularin (**14.2**), 3,4′-dihydroxy-*trans*-stilbene (**14.3**) and 4-hydroxydibenzyl (**14.4**)[30,31] (see Fig. 9). For these stilbenes we recommend adoption of the IUPAC numbering system which uses numbers with primes for the acetate-derived, *meta*-hydroxylated A-ring. Other additions include catabolites of anthranilic acid (**15.1–15.3**)[32,33] (Fig. 9).

The structures of 4′-hydroxyphenylethanol (tyrosol) and 3′,4-dihydroxyphenylethanol (3′-hydroxytyrosol) (**16.1–16.2**) are illustrated in Fig. 10. These phenylethanols are hydrolysis products of oleuropein and presumably of the glycosides which occur in bottle gourd. It has been reported that hydrolysis of oleuropein may occur at gastric pH, independent of the gut microbiota.[34,35] Phase-II metabolites of the phenylethanols (**16.3–16.8**) are also illustrated in Fig. 10.

3. Complications associated with isomers when dealing with microbial and endogenous phenolics and the parent compounds from which they are derived

Regioisomers have the same molecular formula but differ in the sequence in which the atoms are connected. Stereoisomers are not superimposable isomers. They have the same molecular formula and same connectivity but differ in how their atoms are oriented in three-dimensional space. Stereoisomers can be divided into enantiomers and diastereomers. Enantiomers, also known as optical isomers, are non-superimposable mirror images. Diastereomers are stereoisomers which are not mirror images and include, in addition to chiral derivatives, achiral molecules such as symmetrical *meso*-isomers and geometric isomers due to double bond configurations (*cis* and *trans* or *Z* and *E* for the cinnamic acids).

Enantiomers (optical isomers) have the same "scalar" physical properties but opposite "pseudo-scalar" ones such as specific rotation. Regioisomers and diastereomers can have dis-

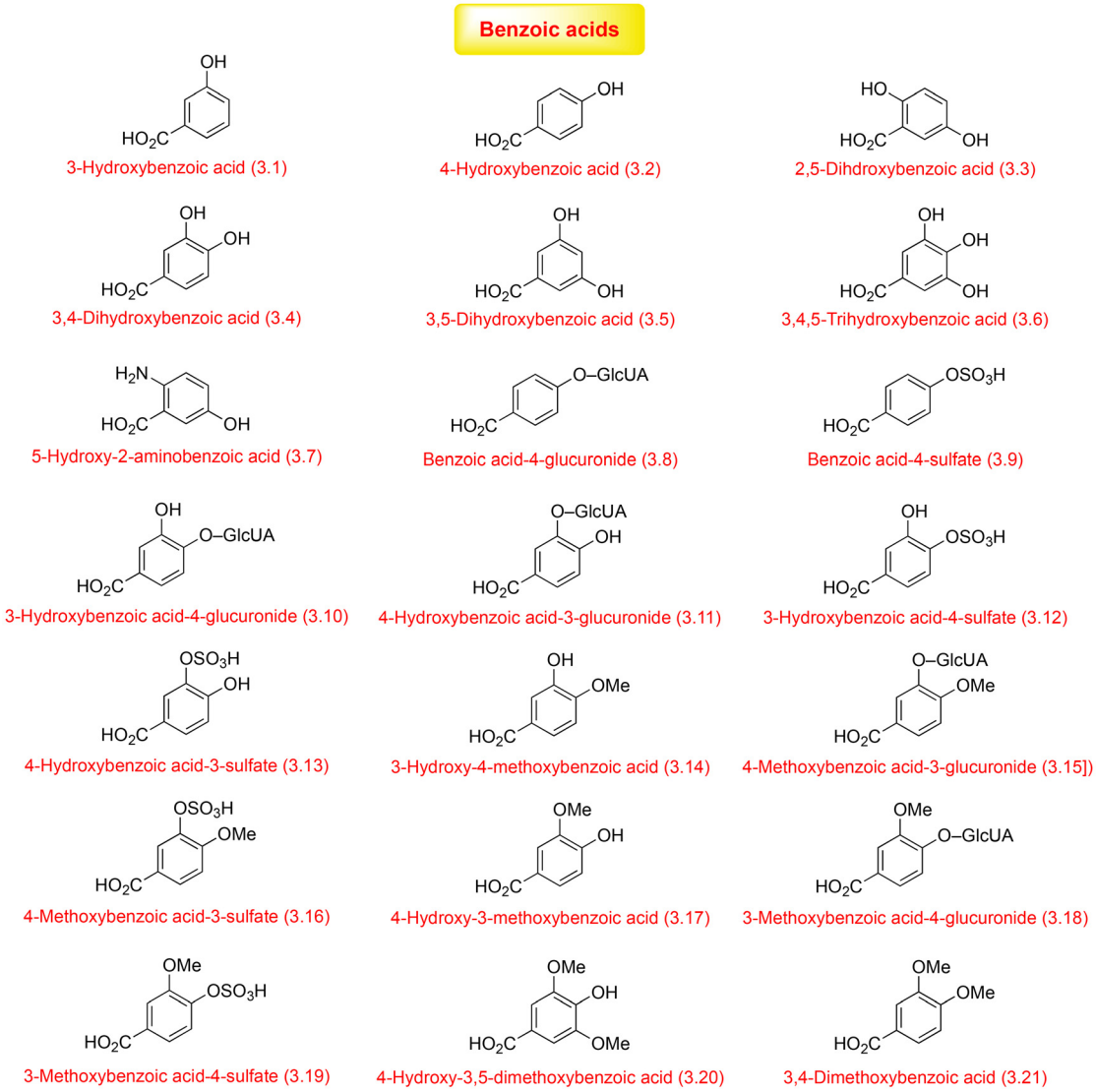

Fig. 2 Structures of benzoic acids (**3.1–3.21**). GlcUA – β-D-glucuronide.

tinct physical and chemical properties, often including different molar absorbance values as well as a different intensity of ionization in mass spectrometry, which potentially can make quantitative estimates of one isomer inaccurate if quantified with the alternative isomer. Regioisomers sometimes have different fragmentation patterns which facilitate identification. Proteins, receptors, and enzymes are chiral biomolecules that discriminate regioisomers and stereoisomers, which can therefore differ in their metabolism and physiological effects.

Enantiomers share the same connectivity but specular 3D-arrangement of atoms: namely, they present opposite "absolute" configuration. Such configuration, usually defined with one or more specific descriptors, such as *R*- or *S*-, which are assigned to every stereogenic element present in the molecule, does not vary with respect to how we rotate the molecule in a plane. Using a γ-valerolactone metabolite as an example, Fig. 11 illustrates how perspective influences the appearance of an enantiomer's 3D structure presented in two dimensions, in this case whether the lactone oxygen projects out from the plane of the page or projects into the plane, and whether the aryl ring is on the right or on the left. Note that the position of the aryl ring does not alter the chirality at C4.

When dealing with pure, chiral bioactive substances, the issue of defining the stereoisomeric composition of the sample is crucial: indeed, two stereoisomers, being diastereo- or enantiomers will also interact differently with another chiral, enantiopure (bio)molecule such as a protein or a sugar, enabling different, sometimes even opposite, (bio)activities. As an example, (*R*)-Ibuprofen (see Fig. 12) does not inhibit prostaglandin synthesis but is metabolized to a CoA-thioester, whereas (*S*)-ibuprofen does not form a CoA-thioester and is an inhibitor of prostaglandin synthesis in humans, with significant enantiomeric differences in human pharmacodynamics.[36,37] Also, (*S*)-ibuprofen is *ca.* 2.5-times more

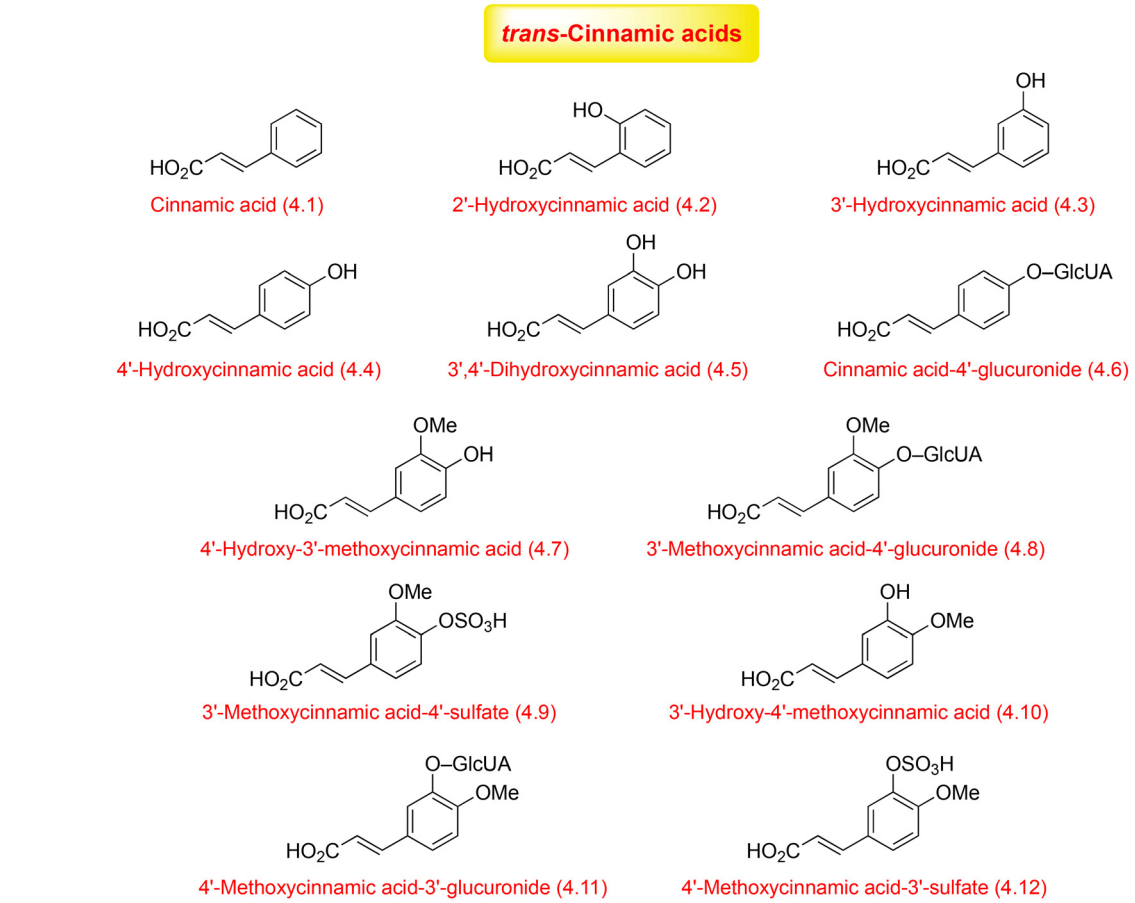

Fig. 3 Structures of *trans*-cinnamic acids (**4.1–4.12**). Cinnamic acids may have *cis* (*Z*) or *trans* (*E*) geometries. In nature the *trans* isomers, which are illustrated, are the more common. GlcUA – β-D-glucuronide.

efficiently absorbed through healthy skin and is a more efficient inhibitor of the human organic anion transporter (*h*OAT1): 2.84 mM for (*S*)-Ibuprofen for 50% inhibition compared with 6.14 mM for (*R*)-Ibuprofen.[38] The (*S*)-isomer is also a slightly more potent inhibitor of lactic acid uptake by the mono-carboxylic acid transporter,[39] and potentially also benzoic acid, 2-hydroxy-, 3-hydroxy and 4-hydroxybenzoic acid. There are also differences in the metabolism of the enantiomers of (*R*/*S*)-2-hydroxy-2-(phenyl)acetic acid in primary rat hepatocytes. The main metabolite of the (2*S*)-enantiomer is phenyl-glyoxylic acid, whereas the (2*R*)-enantiomer yields predominantly benzoic acid and hippuric acid (Fig. 12).[40]

We have located only two publications on the physiological effects of pure phenyl-γ-valerolactone enantiomers.[41,42] Both reports used a numbering system different to that recommended by Kay *et al.*[29] as the heterocyclic lactone oxygen was designated 1 and the centre of chirality was designated 5. For consistency with our recommendations for the various C_6–C_5 metabolites, this has been adjusted in the account which follows with the center of chirality designated 4 (see Fig. 7).

(*S*)-5-(3′,4′-Dihydroxyphenyl)-γ-valerolactone at 25 μmol L^{-1} is slightly more active *in vitro* than its (4*R*)-isomer in protecting rat intestinal epithelial IEC-6 cells against LPS-induced inflammation by inhibiting NF-κB activation.[41] In a second investigation, 1 μmol L^{-1} of the (4*S*)-enantiomer reduced UV-induced MMP-1 protein expression in human dermal fibroblasts by *ca.* 50%, relative to control, whereas the (4*R*)-enantiomer was ineffective.[42] The relative amounts of the (4*R*)- and (4*S*)-enantiomers in the human circulation are not known, but as (+)-catechin and (−)-epicatechin are commonly consumed together, it is likely that both enantiomers will be present.

Mandelic, phenyl-lactic, phenyl-hydracrylic, 4-hydroxy-5-phenylvaleric acids and associated γ-valerolactones are frequently reported metabolites, but apart from the examples given above, the metabolism and physiological effects of their enantiomers have not been compared, and such investigations are required. Many papers present metabolite structures where the 'wiggly' bond is not used to designate a centre of chirality when the chirality is unknown, and this is doubtless one factor which has led to reduced awareness of such isomers and a failure to investigate the associated phenomena. We recommend marking the centre of chirality with an asterisk for racemates or when the absolute configuration is unknown.

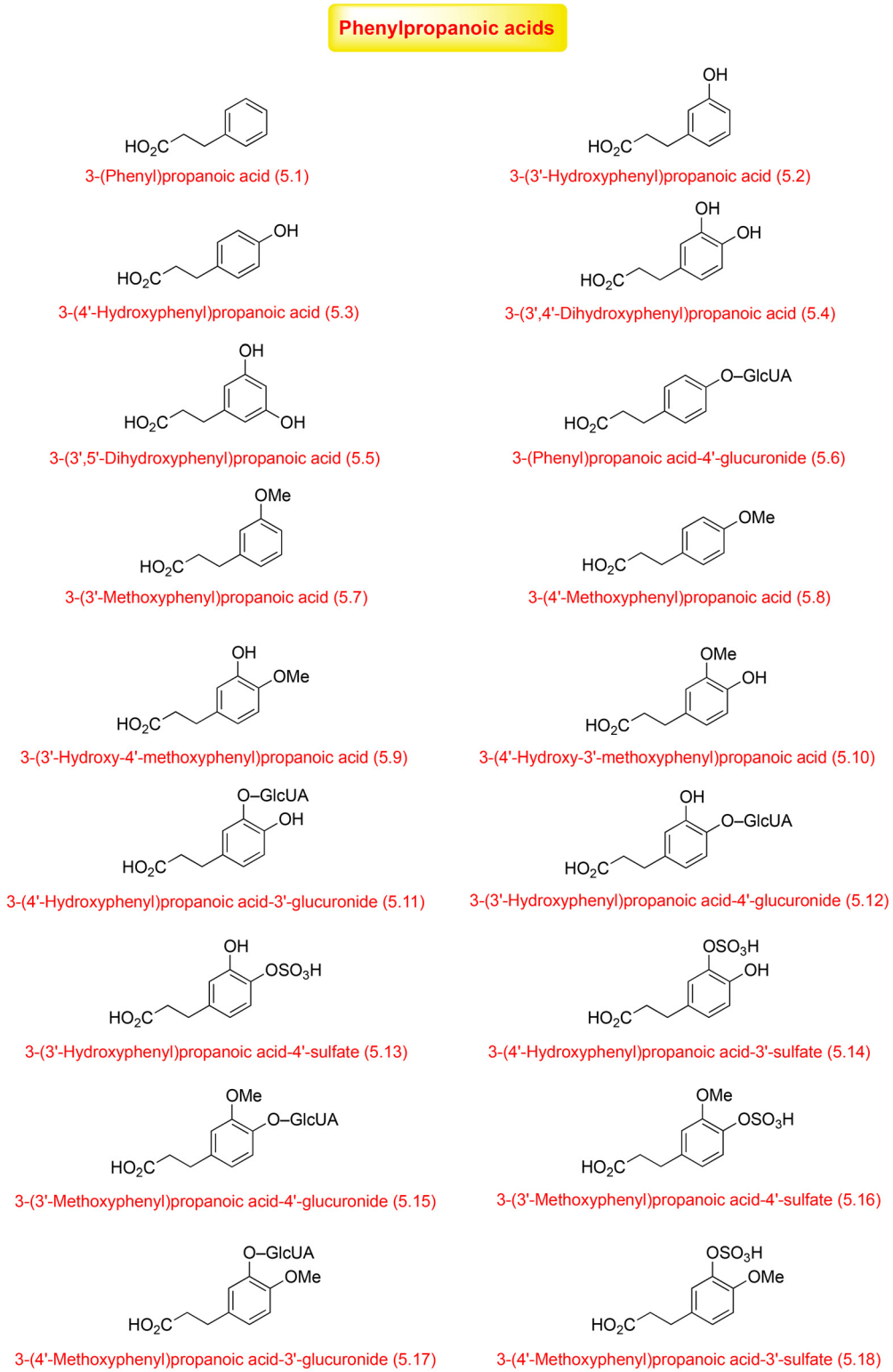

Fig. 4 Structures of (phenyl)propanoic acids (**5.1–5.18**). GlcUA – β-D-glucuronide.

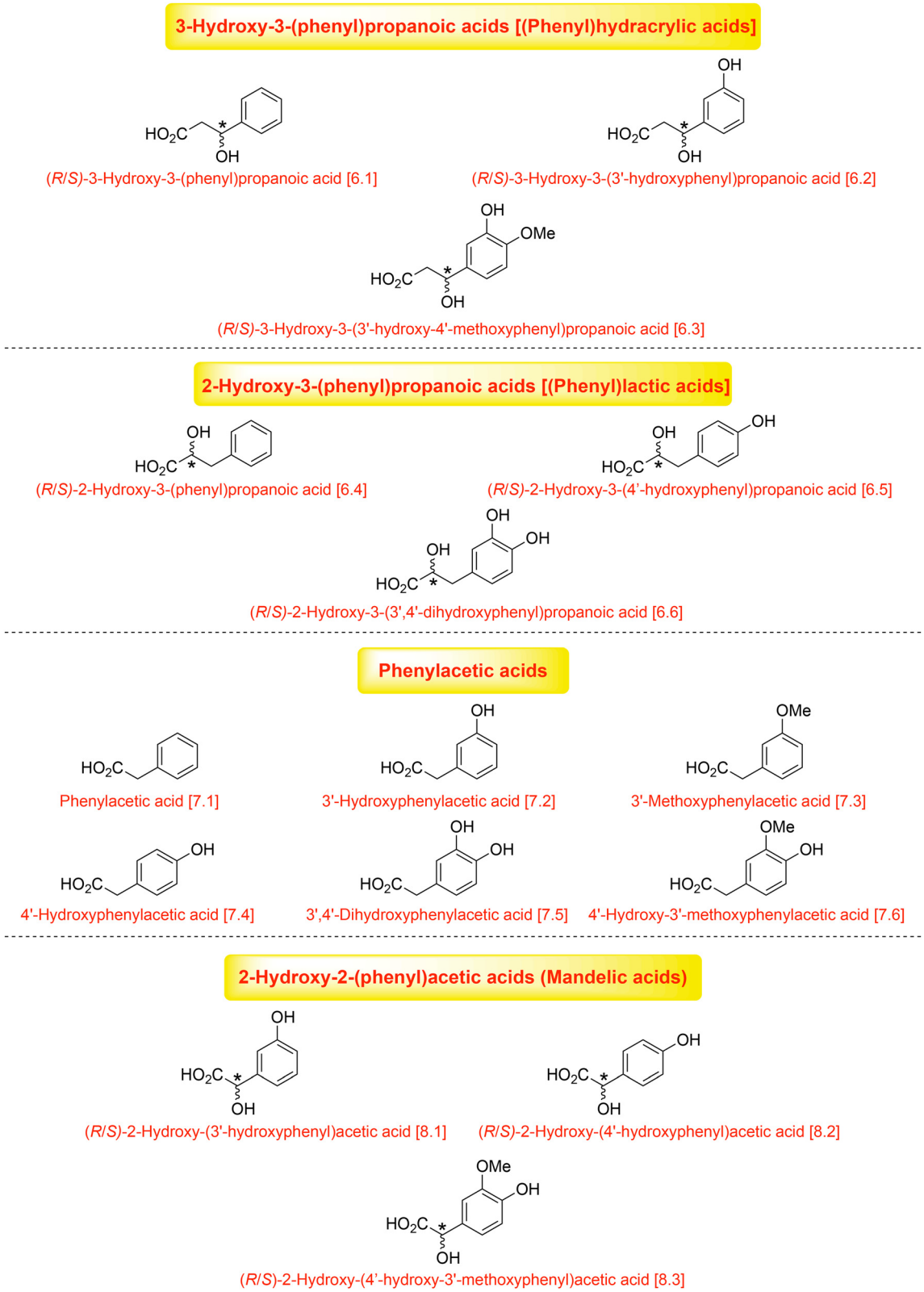

Fig. 5 Structures of 3-hydroxy-(phenyl)propanoic acids (**6.1–6.3**), 2-hydroxy-3-(phenyl)propanoic acids (**6.4–6.6**), phenylacetic acids (**7.1–7.6**) and 2-hydroxy-2-(phenyl)acetic acids (**8.1–8.3**). The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*).

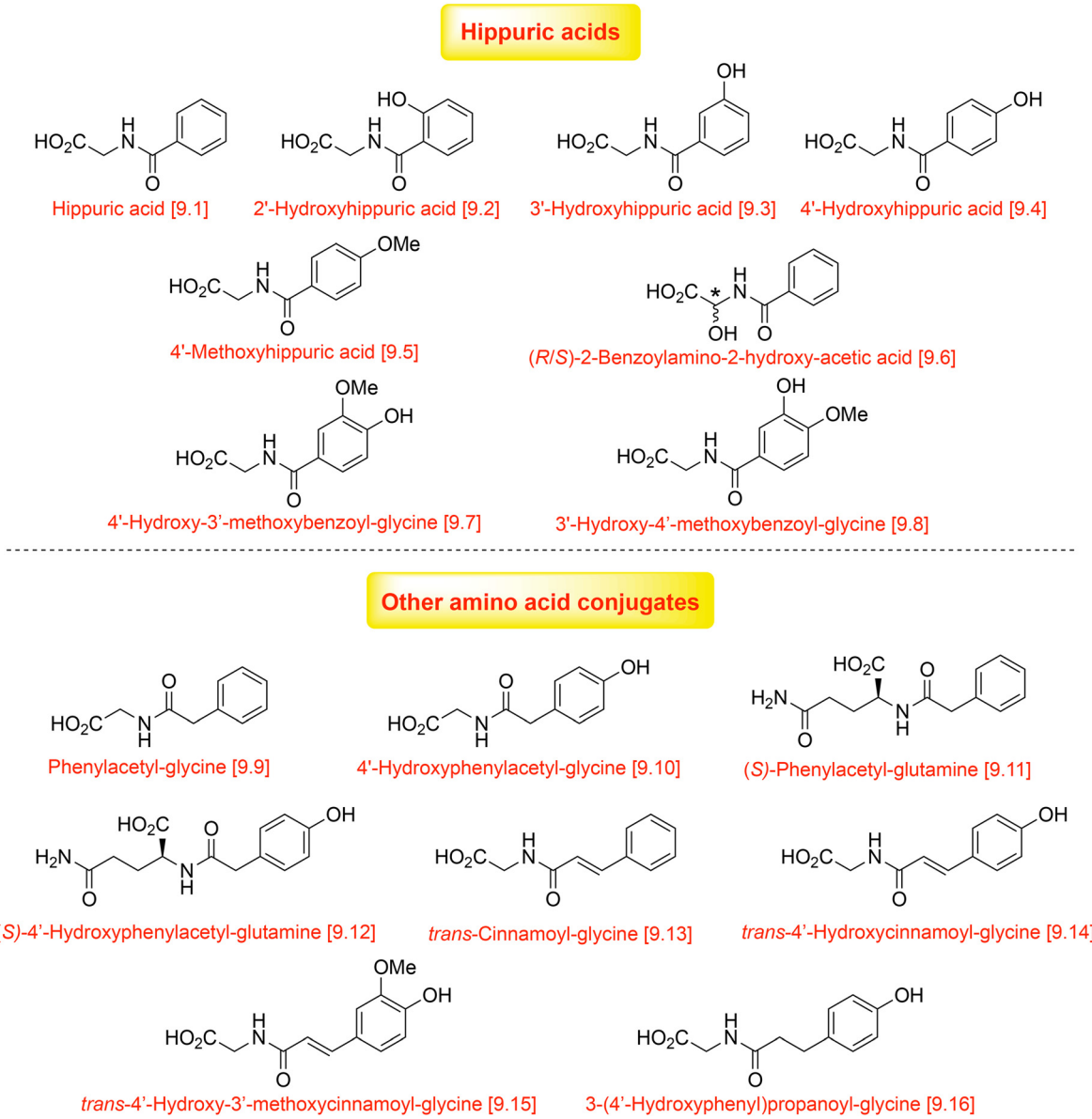

Fig. 6 Structures of hippuric acids (**9.1–9.8**) and other amino acid conjugates (**9.9–9.16**). The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*).

The limited number of commercially available pure enantiomers (see Table 2) and the impossibility of resolving the enantiomers on achiral reversed phase column packings (*i.e.* embedding stationary phases lacking any chiral discriminating groups) exacerbate the problem. Even if a standard of defined stereochemistry is believed to have been used, it does not automatically follow that the sample contains that specific enantiomer as it could be a mixture or merely the alternative enantiomer. To solve this problem, chiral column packings are available, but they are not well suited to the analysis of samples also containing fifty or more achiral metabolites as tedious fraction collection and reanalysis are required to determine if both enantiomers are present. However, in the absence of standards, further investigation is required to fully assign any enantiomer(s) that are detected. Interestingly, when such enantiomers are phase-II conjugated with a chiral, enantiopure β-D-glucuronic acid moiety, as is the norm at least for the C_6–C_5 enantiomers,[43] and possibly for (*R*/*S*)-3-hydroxy-3-(3′-hydroxyphenyl)propanoic acid,[44] the two enantiomers become diastereomers, and as such, they could potentially be resolved on an achiral column packing although we are not aware of any reports of the presence of both isomers and possibly these have been overlooked.

Of note, the resolution of both diastereomers of (*R*/*S*)-3-hydroxy-3-(3′,4′-dihydroxycinnamoyl)quinic acid on an achiral, reversed phase column has been noted: here, the quinic acid

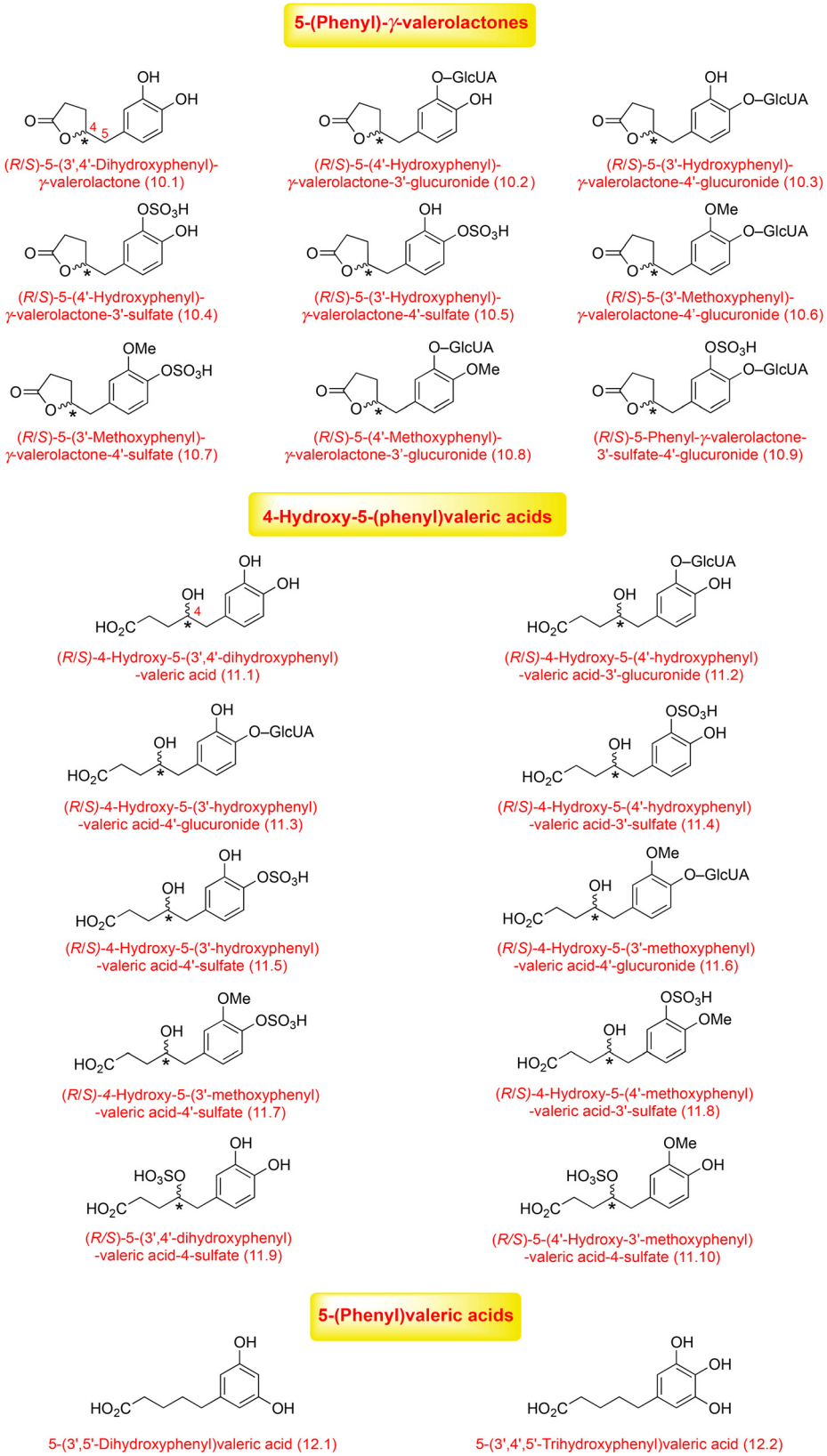

Fig. 7 Structures of 5-(phenyl)-γ-valerolactones (**10.1–10.9**), 4-hydroxy-5-(phenyl)valeric acids (**11.1–11.10**) and 5-(phenyl)valeric acids (**12.1–12.2**). GlcUA – β-D-glucuronide. The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*).

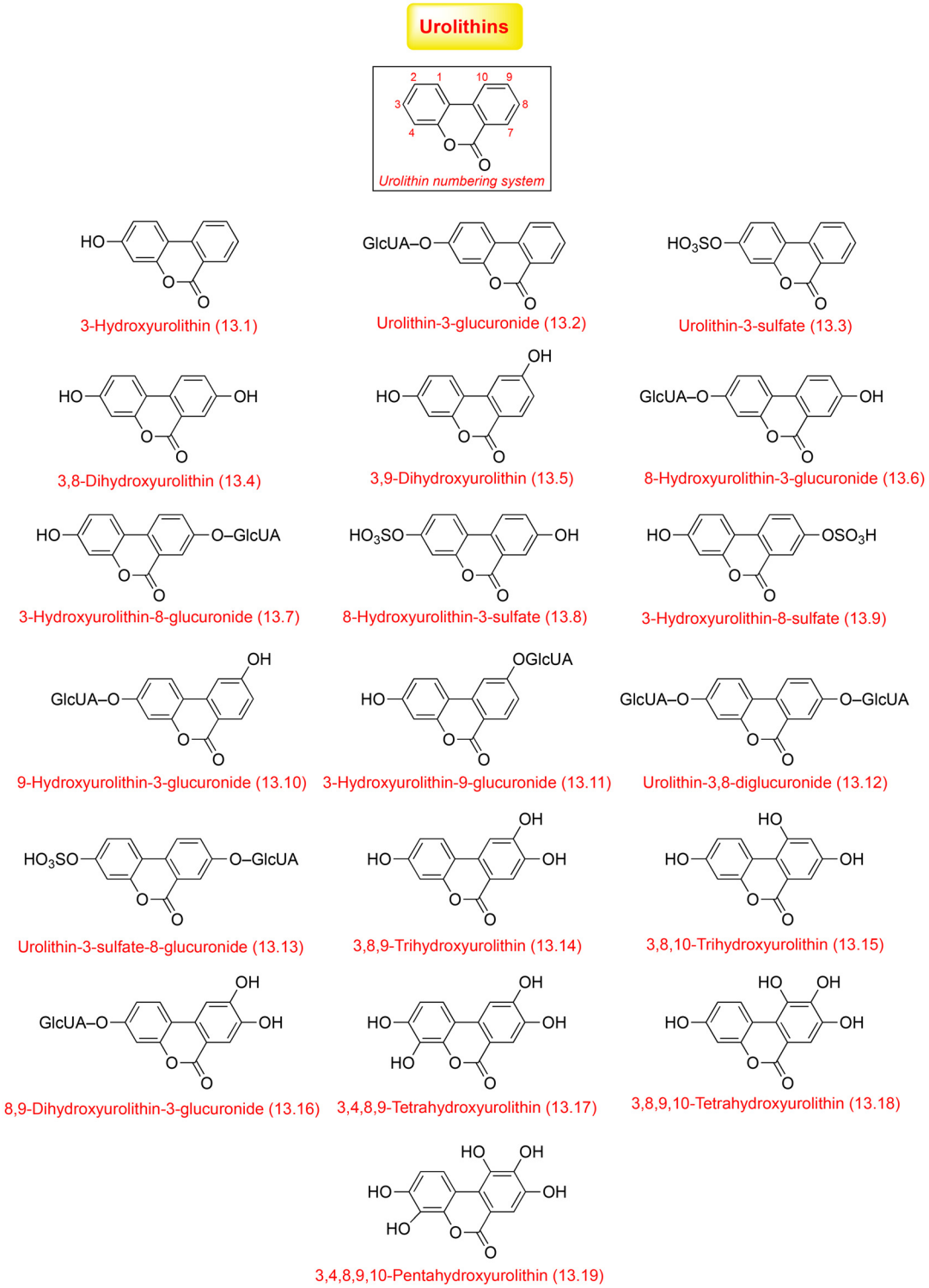

Fig. 8 Structures of urolithins (**13.1–13.19**). GlcUA – β-D-glucuronide.

moiety effectively acted as a covalent chiral resolving agent, enabling the formal separation (identification) of both enantiomers of 3-hydroxy-3-(3′,4′-dihydroxyphenyl)cinnamic acid.[45] This indicates that a similar resolution of the C_6–C_5-glucuronide conjugates is feasible.

3.1. C_6–C_5 phenyl-γ-valerolactones and phenyl-valeric acids

As stated above, few pure enantiomers are available, and vendors' catalogues can be confusing and may sometimes be incorrect. For example, the Shanghai Ichemical

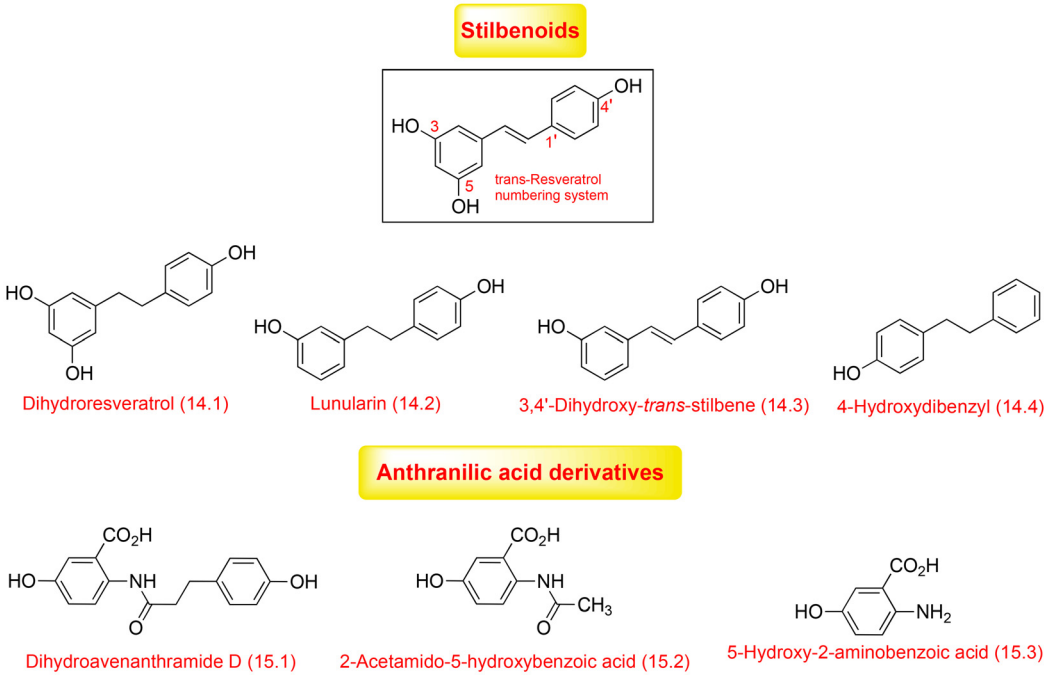

Fig. 9 Structures of stilbenoids [**14.1–14.4**] and anthranilic acid derivatives [**15.1–15.3**].

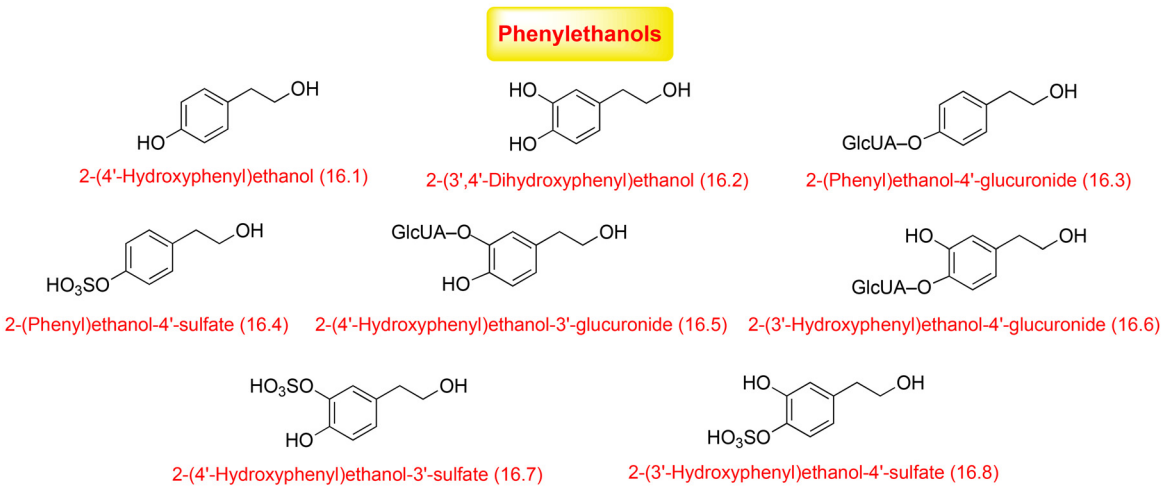

Fig. 10 Structures of phenylethanols [**16.1–16.8**]. GlcUA – β-D-glucuronide.

Co., Ltd‡ refer to the CAS Registry number 21618-92-8 for their product (*S*)-5-(3′,4′-dihydroxy)phenyl-γ-valerolactone, whereas Toronto Research Chemicals§ use CAS Registry number 191666-22-5 for the same compound and both suppliers provide the correct structure for the listed isomer on their website. In contrast, many other suppliers, for example Alfa Chemistry¶, use an enantiomerically undefined structure for 21618-92-8, possibly suggesting that their material is uncharacterized or racemic despite using the (4*S*) CAS Registry number. Santa Cruz Biotechnology‖ provide no structure for 191666-22-5 but its explicit description as a '*minus-epicatechin-metabolite*' implies that it is the (4*R*)-isomer. Fig. 13 illustrates the relationship between (+)-catechin and (−)-epicatechin and the

‡ https://www.ichemical.com/products/21618-92-8.html
§ https://www.trc-canada.com/product-detail/?D454525
¶ https://www.chemicalbook.com/ProdSupplierGWCB21302752_EN.htm
‖ https://www.scbt.com/p/4r-5-3prime-4prime-dihydroxyphenyl-gamma-valerolactone-minus-epicatechin-metabolite-191666-22-5

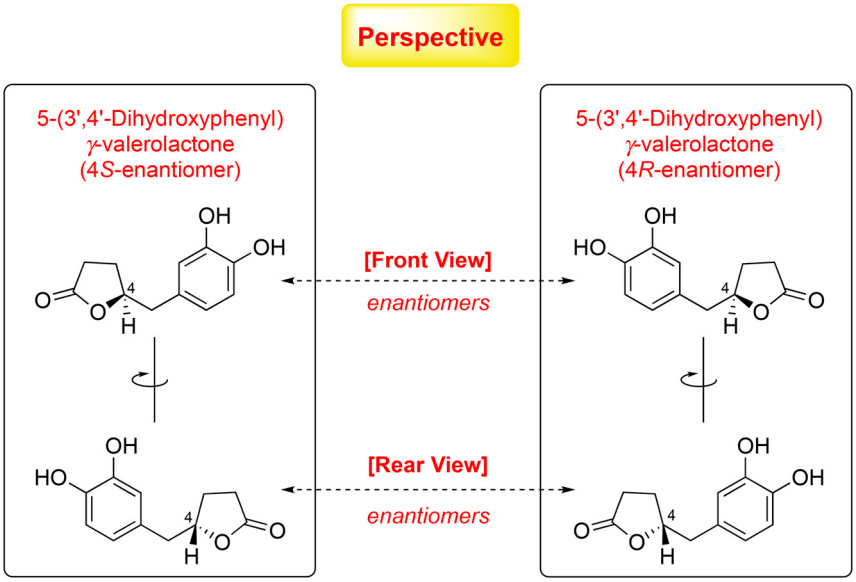

Fig. 11 Structures of the (4*S*)- and (4*R*)-enantiomers of 5-(3,4-dihydroxyphenyl)-γ-valerolactone from a front and rear perspective.

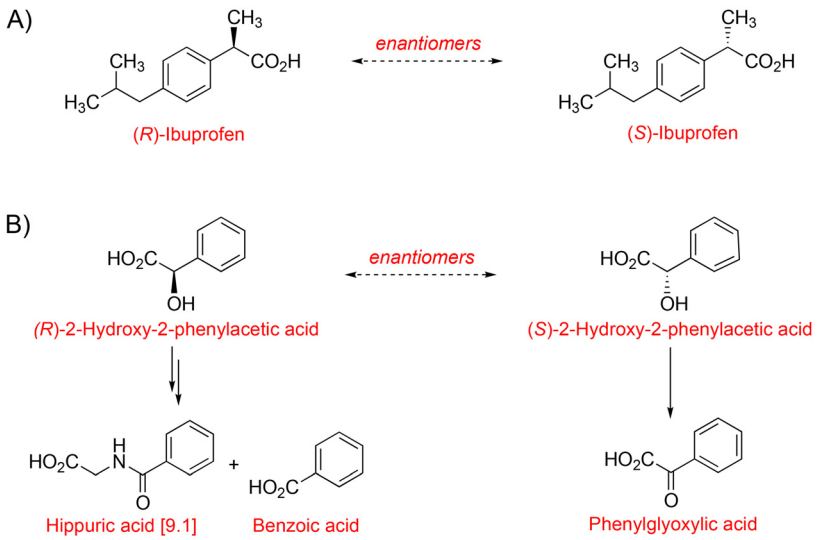

Fig. 12 (A) Structures of (*R*)- and (*S*)-ibuprofen (2-(4′-isobutyl-phenyl)propanoic acid aka isobutylphenylpropionic acid) and (B) the differential metabolism of (*R*)- and (*S*)-2-hydroxy-2-(phenyl)acetic acid by primary rat hepatocytes.

associated phenyl-γ-valerolactone and phenyl-valeric acid gut microbiota catabolites. It is not known whether there is a mammalian racemase enzyme interconverting (*R*)- and (*S*)-forms for these C_6–C_5 lactones and acids.

To confound the confusion, Phytohub** lists three CAS numbers, 21618-92-8, 191666-22-5 and 1108192-01-3, all for a compound described as "5-(3′,4′-dihydroxyphenyl)-γ-valerolactone". CAS 1108192-01-3 is also used by the Royal Society of Chemistry's Chemspider†† which lists 11 suppliers, all of whom associate it with the structure having undefined stereochemistry.

** https://phytohub.eu/entries/PHUB001993

†† https://www.chemspider.com/Chemical-Structure.134347.html?rid=d203472f-cd06-48d1-ab43-18cd7d078353

Table 2 Commercially available enantiomers[b]

CAS Number	Recommended name	Supplier[a]	Supplier's webpage
C_6–C_5 acids and lactones			
21618-92-8	(*S*)-4-Hydroxy-5-(3′,4′-dihydroxy)phenyl-γ-valerolactone	1	**https://www.ichemical.com/products/21618-92-8.html**
191666-22-5	(*R*)-4-Hydroxy-5-(3′,4′-dihydroxy)phenyl-γ-valerolactone	2	**https://www.trc-canada.com/product-detail/?D454525**
1190403-76-9	(*R*)-4-Hydroxy-5-(3′,4′-dihydroxyphenyl)valeric acid	2	**https://www.trc-canada.com/product-detail/?D454580**
Mandelic acids			
17119-29-0	(*S*)-2-Hydroxy-2-(phenyl)acetic acid	3	**https://ambeed.com/products/17119-15-2.html**
611-71-2	(*R*)-2-Hydroxy-2-(phenyl)acetic acid	4	**https://www.sigmaaldrich.com/GB/en/search/611-71-2?focus=products&page=1&perpage=30&sort=relevance&term=611-71-2&type=cas_number**
90-64-2	(*R*/*S*)-2-Hydroxy-2-(phenyl)acetic acid undefined	4	**https://www.sigmaaldrich.com/GB/en/search/90-64-2?focus=products&page=1&perpage=30&sort=relevance&term=90-64-2&type=cas_number**
13244-78-5	(*R*)-2-Hydroxy-2-(4′-hydroxyphenyl)acetic acid	3	**https://ambeed.com/products/17119-15-2.html**
Phenyl-hydracrylic acids			
2768-42-5	(*R*)-3-Hydroxy-3-(phenyl)propanoic acid	5	**https://www.fishersci.com/shop/products/r-3-hydroxy-3-phenylpropionic-acid-98-thermo-scientific/AAL19040MD**
36567-72-3	(*S*)-3-Hydroxy-3-(phenyl)propanoic acid	4, 6	**https://www.sigmaaldrich.com/GB/en/product/aldrich/56193** **https://www.thermofisher.com/order/catalog/product/L19041.03**
Phenyl-lactic acids			
7326-19-4	(*R*)-2-hydroxy-3-(phenyl)propanoic acid	7	**https://www.aechemsc.com/info_products/AE1-008987.php**
20312-36-1	(*S*)-2-hydroxy-3-(phenyl)propanoic acid	8	**https://www.selleckchem.com/products/s-2-hydroxy-3-phenylpropanoic-acid.html**
828-01-3	(*R*/*S*)-2)-hydroxy-3-(phenyl)propanoic acid	9	**https://www.simsonpharma.com/product/dl-2-hydroxy-3-phenylpropionic-acid**

[a] 1 – Shanghai Ichemical Co., Ltd; 2 – Toronto Research Chemicals; 3 – Ambeed; 4 – Sigma Aldrich; 5 – Fischer Scientific; 6 – ThermoFischer Scientific; 7 – AEChem Scientific Corporation; 8 – SelleckChem.com; 9 – SimSon Pharma Ltd. [b] This table was prepared purely for the convenience of readers and the authors have no connection with these companies and make no claims regarding the quality of the materials they supply. There may be other providers and compendia such as Chemspider **https://www.chemspider.com/** and Pubchem **https://pubchem.ncbi.nlm.nih.gov/** should also be consulted, particularly for the racemates.

3.2. The enantiomeric mandelic, phenyl-hydracrylic, phenyl-lactic and hydrotropic acids

3.2.1. Mandelic acids. Mandelic acids such as (*R*/*S*)-2-hydroxy-2-(phenyl)acetic acid are often sold as *racemic compounds* known to contain both enantiomers and such preparations should be identified by the prefix '*rac*'. The designated structures are illustrated in Fig. 14. It is of note, however, that there is a difference between a preparation that is known to be a '*racemate*' and a preparation or chromatographic peak of 'unknown chirality', which might be a single isomer or a mixture of both enantiomers.

(*S*)-Mandelic acid is epimerized by humans but the enzyme responsible has not been identified. It is not the 2-arylpropanoyl-CoA epimerase (EC 5.1.99.4) which accepts ibuprofen and the isoflavone metabolite (*R*)-2-hydroxy-2-(4′-hydroxyphenyl)propanoic acid.[46]

Matrix Fine Chemicals have an entry on their website‡‡ for '*rac*-(2*R*)-2-hydroxy-2-(4-hydroxyphenyl)acetic acid' which is internally inconsistent with '*rac*' indicating racemic and '2*R*' implying enantiomeric purity. Prospective purchasers who require a specific enantiomer are advised to obtain written confirmation of the identity of the product offered before making an expensive purchase.

3.2.2. Phenyl-hydracrylic acids. In 1957 Armstrong *et al.*[47] reported the presence of a phenyl-hydracrylic acid described as "(−)-*3-hydroxy-3-(phenyl)propanoic acid*" in human urine. They determined the (−)-rotation but did not assign *R*/*S*. There is no direct and predictable relationship between the optical activity and the arrangement of the substituents around the center of chirality (see Fig. 15). This must be determined experimentally on a case-by-case basis. The (+)-optical isomer is now available commercially,§§ and is the (*R*)-enantiomer, indicating that the Armstrong *et al.* isolate must be (−)-(*S*)-3-hydroxy-3-(phenyl) propanoic acid. This enantiomer would be expected for a metabolite produced by mitochondrial β-oxidation.[48] However, it is not known if there is a mammalian racemase enzyme for phenyl-hydracrylic acids. It is of note that the β-oxidation-associated racemase requires at least four carbons in the side chain and, thus, cannot accommodate the phenyl-hydracrylic acid.[48]

3.2.3. Phenyl-lactic acids. Both enantiomers of the phenyl-lactic acids such as (*R*/*S*)-2-hydroxy-3-(phenyl)propanoic acid (Fig. 16) can be expected in human plasma and urine because some anaerobes, for example *Clostridium sporogenes*, convert L-phenylalanine to (*R*)-2-hydroxy-3-phenylpropanoic acid[49] while (*S*)-2-hydroxy-3-(4′-hydroxyphenyl)propanoic acid is an endogenous metabolite of L-tyrosine (Fig. 17).[50] Again, it is not known whether there is a mammalian racemase enzyme for phenyl-lactic acids.

3.2.4. Hydrotropic acids. (*R*/*S*)-2-(Phenyl)propanoic acids are C_6–C_3 phenolics with a methyl group at C2 on the side

‡‡ **https://www.matrix-fine-chemicals.com/products/catalog/secondary-alcohols/mm1704**

§§ **https://www.fishersci.co.uk/shop/products/r-3-hydroxy-3-phenylpropionic-acid-98-thermo-scientific/11349575**

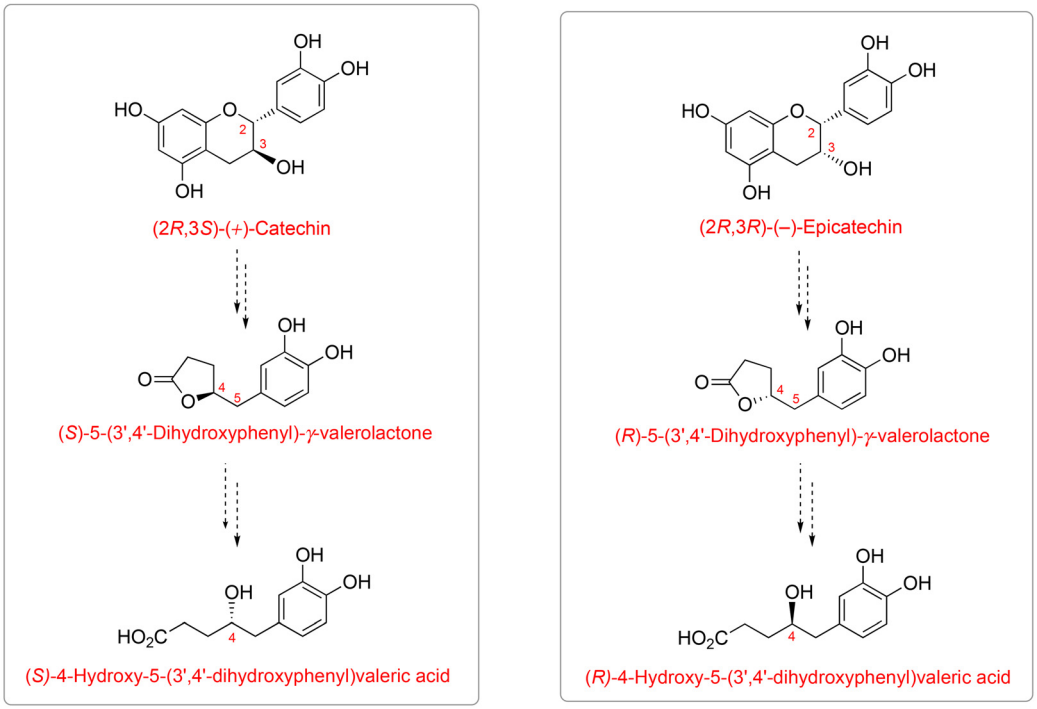

Fig. 13 The relationship between (+)-catechin and (−)-epicatechin and their associated phenyl-γ-valerolactone and phenyl-valeric acid gut microbiota catabolites. The structures viewed from the front are usually preferred in publications.

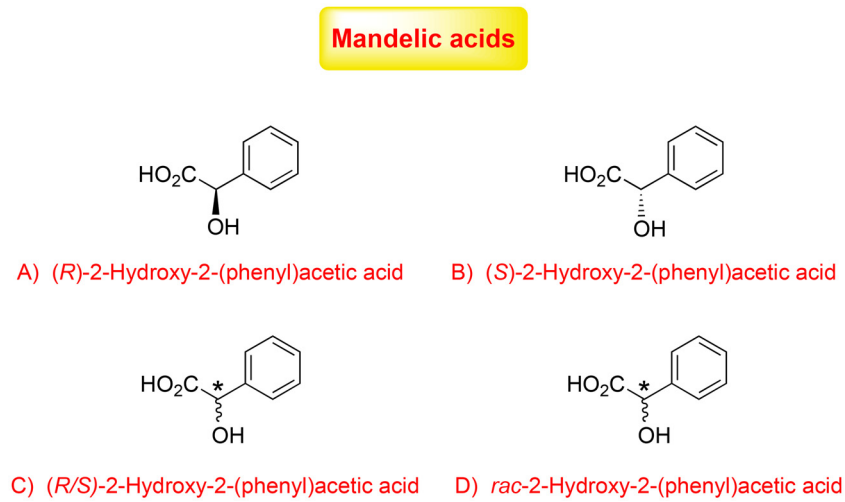

Fig. 14 (*R*)-, (*S*)- and (*R*/*S*)- and *rac*-mandelic acids. (A) (*R*)-enantiomer, (B) (*S*)-enantiomer, (C) (*R*/*S*)- a compound of unknown chirality which might prove to be a mixture of both enantiomers, (D) '*rac*'- a preparation known to contain both enantiomers. The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*). Phenyl ring substituents do not alter the chirality, but the CAS Registry number will change.

chain and are referred to as hydrotropic acids. (*R*)-2-Phenylpropanoic acids are produced from isoflavones by gut microbiota[51] and can be racemized by human α-methylacyl-CoA racemase (2-aryl-propanoyl-CoA epimerase; EC 5.1.99.4).[46] Achiral 3-phenylpropanoic acids with various phenyl ring substituents (Fig. 4) are produced from most other flavonoids, including flavan-3-ols and proanthocyanidins. The structures of the different types of (phenyl)propanoic acids are illustrated in Fig. 18.

3.3. Cinnamic acids

Cinnamic acids occur *in planta* predominantly as *trans*-isomers that are readily converted to *cis*-isomers when exposed to UV light (Fig. 19),[52] and are increasingly being

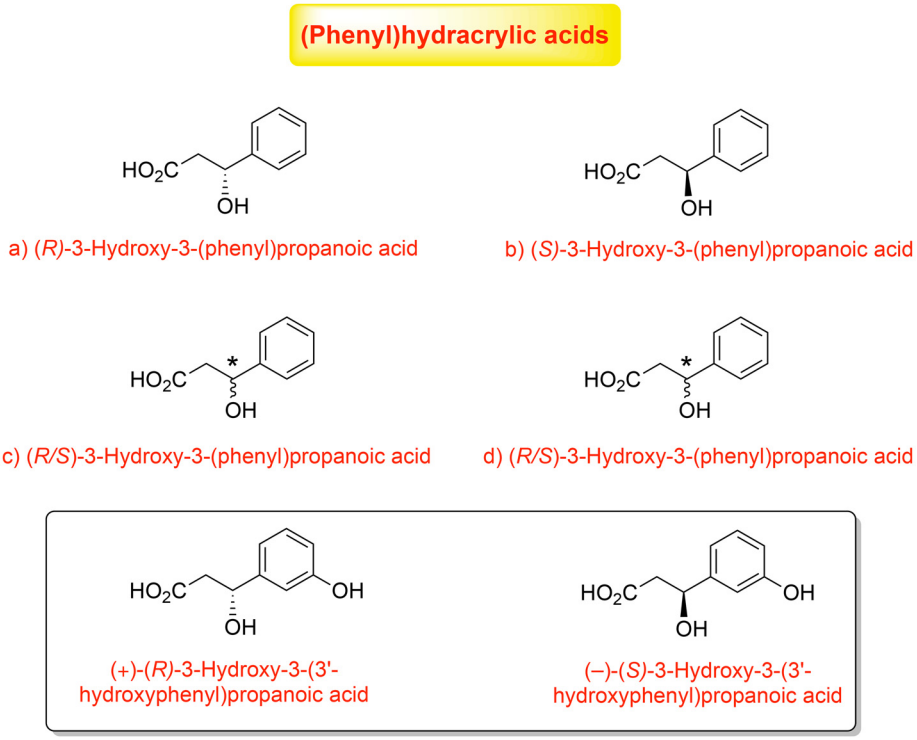

Fig. 15 (*R*)-, (*S*)- and (*R*/*S*)- and *rac*-(phenyl)hydracrylic acids. (a) (*R*)-enantiomer, (b) (*S*)-enantiomer, (c) (*R*/*S*)- a compound of unknown chirality which might prove to be a mixture of both enantiomers, (d) '*rac*'- a preparation known to contain both enantiomers. The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*). Phenyl ring substituents do not alter the chirality, but the CAS Registry number will change. In the box: the two enantiomers of (3'-hydroxyphenyl)hydracrylic acid: the (–)-*S*-enantiomer was found in urine.[45]

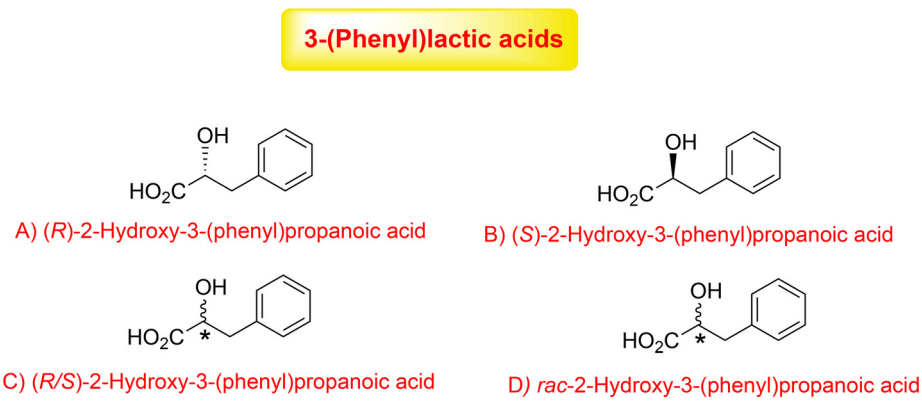

Fig. 16 (*R*)-, (*S*)- and (*R*/*S*)- and *rac*-3-(phenyl)lactic acids. (A) (*R*)-enantiomer, (B) (*S*)-enantiomer, (C) (*R*/*S*)- a compound of unknown chirality which might prove to be a mixture of both enantiomers, (D) '*rac*'- a preparation known to contain both enantiomers. The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*).

reported in leafy tissues, flowers and the surface tissues of fruit and vegetables. *cis*-Isomers have been detected in human feces and urine, possibly preformed before consumption.[53–55] There is evidence for metabolic *trans* to *cis* isomerization by (i) rats,[56] (ii) *Lactobacillus reuteri*, a component of the human gut microbiota,[57] (iii) everted rat gut sacs, and (iv) Caco-2/HT29-MTX co-cultures where a putative *cis*-3′-methoxycinnamic acid-4′-glucuronide (Fig. 19) has been detected.[58] In such circumstances, nomenclature should follow the existing recommendations of Kay *et al.*[29] repeated in the present document (Table 1) but replacing '*trans*' with '*cis*'.

3.4. Hippuric acids

4′-Hydroxy-hippuric acid has a single CAS registry number, 2482-25-9, and along with other hippuric acids, elutes as a

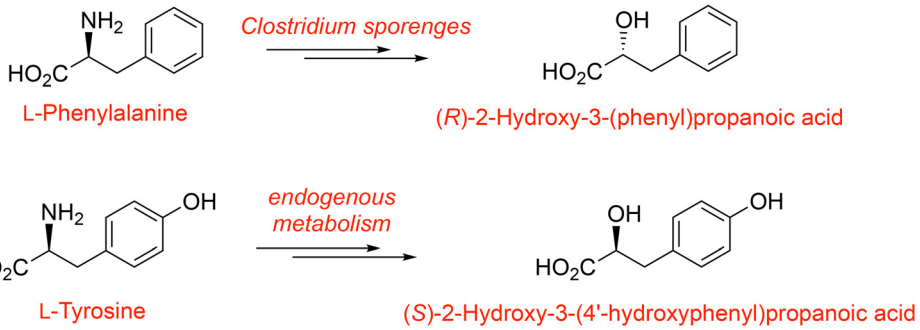

Fig. 17 Gut microbiota metabolites of L-phenylalanine and endogenous metabolites of L-tyrosine.

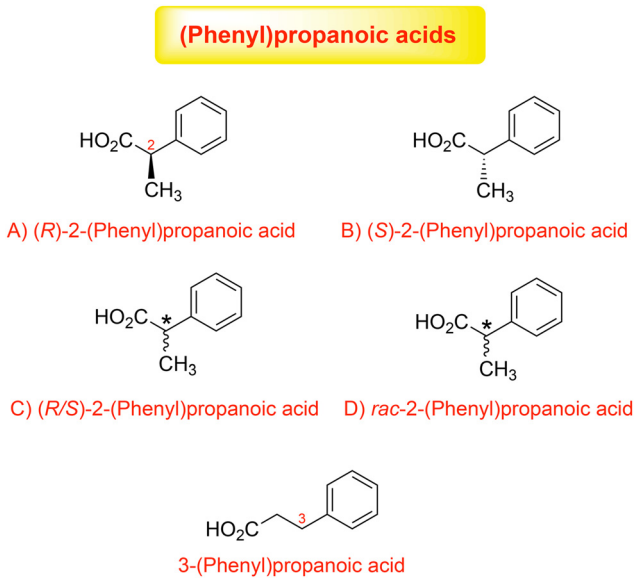

Fig. 18 Chiral 2-(phenyl)propanoic acids (aka hydrotropic acids) and achiral 3-(phenyl)propanoic acids are catabolites of several flavonoids. (A) (*R*)-enantiomer, (B) (*S*)-enantiomer, (C) (*R*/*S*)- a compound of unknown chirality which might prove to be a mixture of both enantiomers, (D) *'rac'*- a preparation known to contain both enantiomers The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*), (E) a chiral 3-(phenyl)propanoic acid.

single peak from reversed phase HPLC column packings. However, after derivatization for GC–MS analysis, hippuric acids typically form two peaks, the amide- and imidic acid-tautomers. The relative yields depend on the derivatizing agent and conditions, as well as the position of the equilibrium associated with each hippuric acid, and areas of both peaks must be utilized in quantitative studies.[59] The amide-tautomer is derivatized on the carboxyl whereas the imidic acid-tautomer is derivatized on the carboxyl and the side chain hydroxyl, plus, for both tautomers, any hydroxy groups attached to the ring (Fig. 20).[59]

3.5. Glutathione conjugates

One of the actions of the tripeptide glutathione (L-γ-glutaminyl-L-cysteinyl-glycine) (Fig. 21) is to scavenge electrophilic species, often toxicants or potential toxicants, such as the quinones generated by cytochrome P450 2E1 and 3A4 from phenolic metabolites of dietary or pharmaceutical origin (for example paracetamol aka acetaminophen, and *N*-(4′-hydroxyphenyl)acetamide) (Fig. 21). Scavenging may occur enzymically *via* glutathione-*S*-transferase (EC 2.5.1.18), or by purely chemical interaction such as addition to the

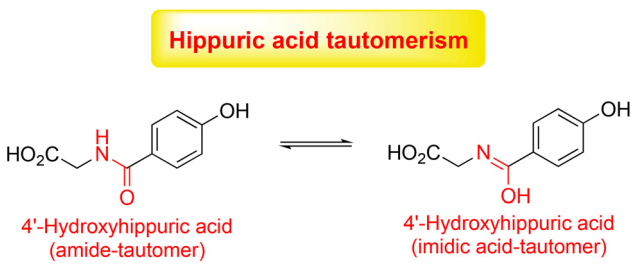

Fig. 20 The amide- *vs.* imidic acid-tautomer of 4′-hydroxyhippuric acid.

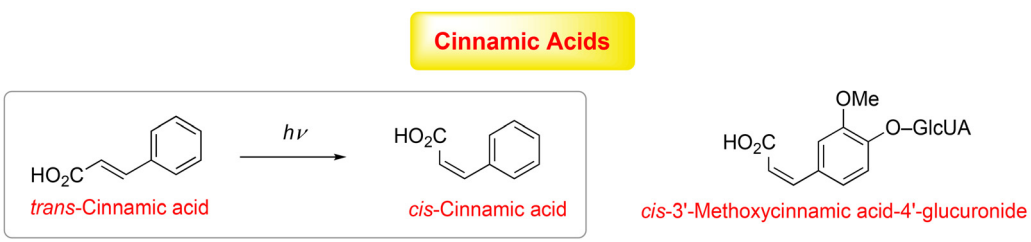

Fig. 19 *trans*- and *cis*-cinnamic acid and *cis*-3′-methyoxycinnamic acid-4′-glucuronide. GlcUA – β-D-glucuronide, *hv* – UV irradiation.

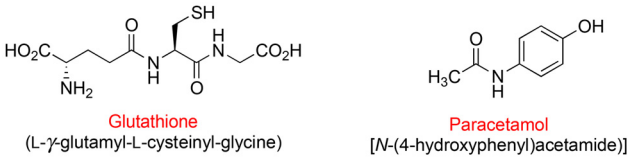

Fig. 21 Glutathione and paracetamol.

α,β-conjugated double bond of cinnamic acids.[60] Such conjugates may be undetectable at normal dietary (poly)phenol intake but have been observed after experimental diets rich in (poly)phenols[61] and, based on animal and *in vitro* studies, they may be increased under conditions of oxidative stress and/or when catechol-*O*-methyl transferase (EC 2.1.1.6) activity is impaired.[62] *In vivo* conjugation is followed by hydrolysis of the glutathione moiety yielding the cysteinyl conjugate which is *N*-acetylated producing the mercapturic acid conjugate. Glutathionyl-conjugates are usually excreted in bile whereas the mercapturic acid conjugates are generally excreted in urine.

Note that glutathione conjugates of caffeoylquinic acids and caftaric acids may also occur in foods and wine,[63,64] but their presence in biological fluids at a normal dietary (poly)phenol intake could be more related to hepatic conjugation rather than direct absorption at gastrointestinal level. Indeed, single mercapturic acid conjugates of 3-(3′,4′-dihydroxyphenyl)propanoic acid, 3,4-dihydroxybenzaldehyde and 1,2-dihydroxy-4-methylbenzene, plus two isomeric conjugates of 3′,4′-dihydroxyphenylacetic acid, and three isomeric conjugates of 3′,4′-dihydroxycinnamic acid have been detected in urine after volunteers consumed 200 g cooked onion containing *ca.* 250 μmoles of quercetin glycosides.[61] This bolus intake from onions is approximately an order of magnitude higher than the typical human daily consumption of quercetin glycosides from all sources throughout the day.

In vitro studies with 3′,4′-dihydroxycinnamic acid indicate that glutathione conjugation may occur at C2′, C5′ and C6′ on the phenyl ring, and at C3 of the side chain, theoretically producing two diastereomers, although whether both are formed is not known. The phenyl ring conjugates can be assigned to regioisomers only by NMR, but the benzylic side chain conjugates are saturated and distinguishable by their increased mass and fragmentation.[62,63,65] Hence it might be possible to distinguish between the aromatic mercapturic acid adducts of 3-(3′,4′-dihydroxyphenyl)propanoic acid (M_r – 343.07257 amu) and the benzylic mercapturic acid adduct of 3′,4′-dihydroxycinnamic acid, (M_r – 341.05692 amu) (Fig. 22). Until authentic glutathione and mercapturic acid conjugates are available, or such phenyl-ring adducts are isolated and fully characterised, these metabolites can only be described as mercapturic acid (glutathionyl) conjugates of X, where X is described using the recommendations already established.

3.6. Lignans and enterolignans

Several classes of lignans and enterolignans are illustrated in Fig. 23 and 24. Secoisolariciresinol can occur as a pair of C_2-symmetric, optically active enantiomers as well as an optically inactive symmetrical *meso*-isomer (Fig. 23). The optically active (2*R*,3*R*)-lignans are predominant in foods. Zálešák *et al.*[66] listed 10 classes of lignans and 15 classes of neolignans, all of which originate *in planta* from the dimerization of two *trans*-cinnamoyl alcohol moieties which are commonly glycosylated on the side chain alcohols. The human gut microbiota catabolism of five classes of lignans associated

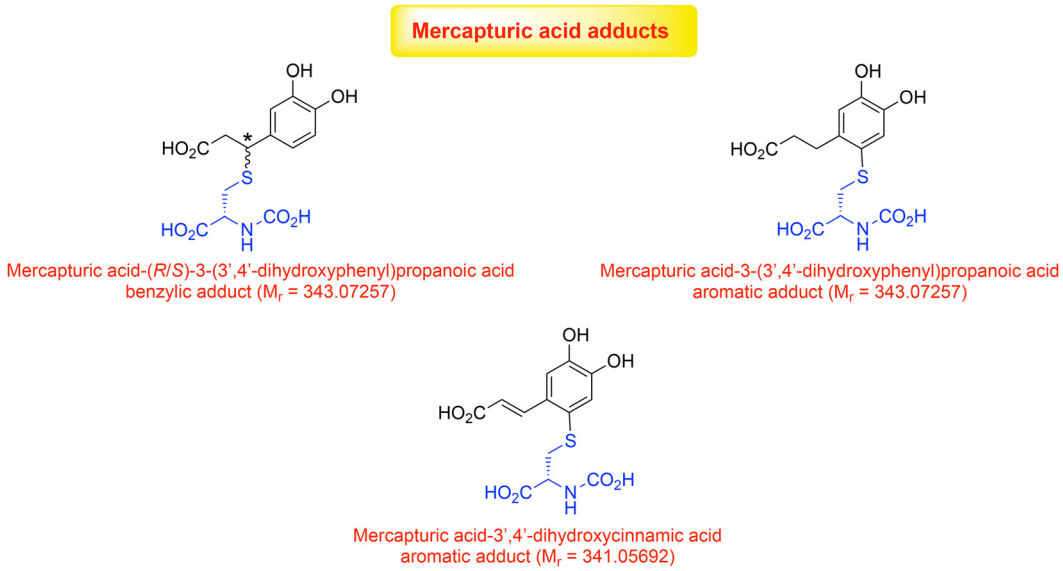

Fig. 22 Benzylic (black) and aromatic mercapturic acid (blue) adducts. The asterisk "*" represents the presence of a chiral centre of unknown absolute configuration (*R* or *S*).

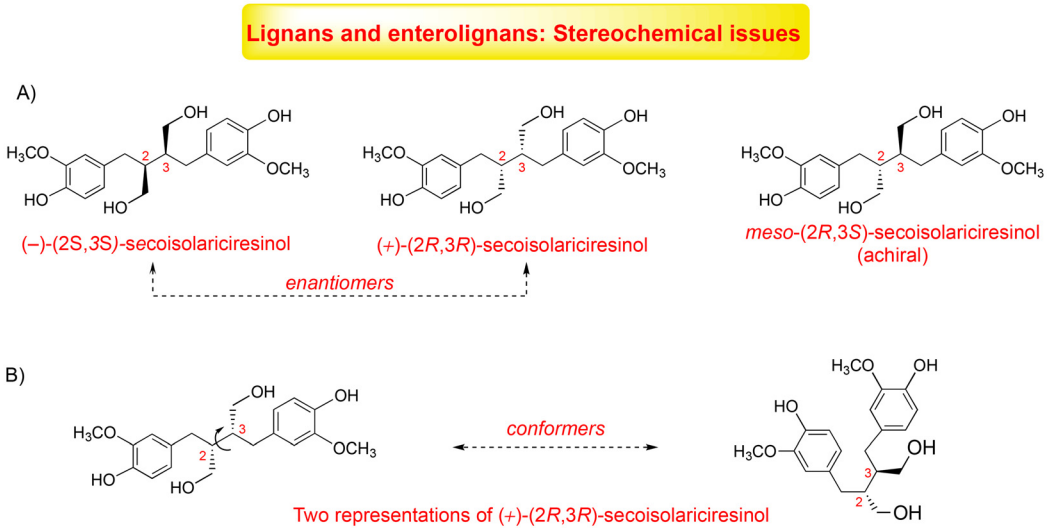

Fig. 23 (A) The structure of lignan diastereomers illustrated using secoisolariciresinol as an example. (B) Representation of two conformations of (+)-(2*R*,3*R*)-secoisolariciresinol unveiling its C_2-symmetry pattern.

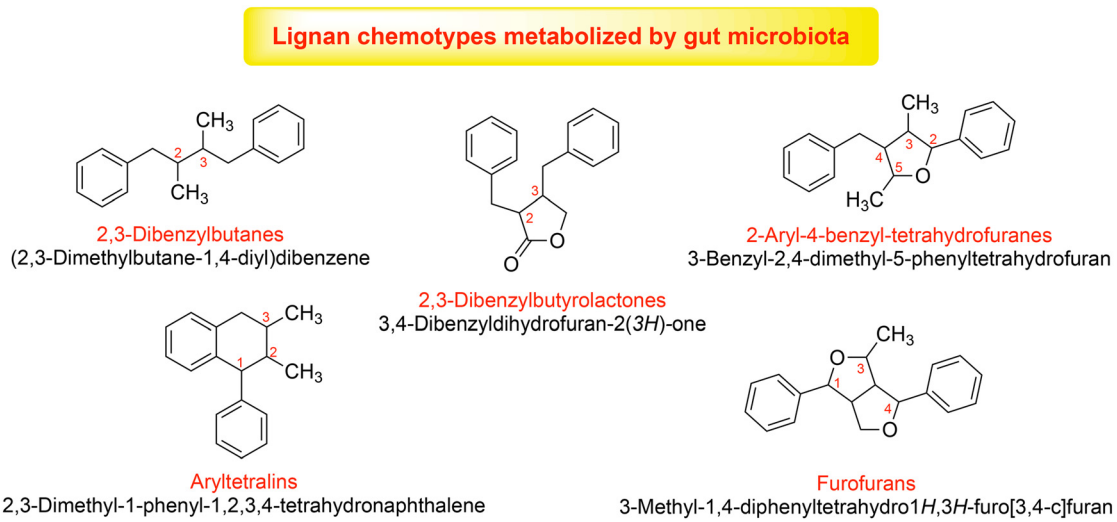

Fig. 24 Skeleton structures of the five classes of lignans of which the gut microbiota catabolism has been investigated. Red names – synonyms; black – IUPAC nomenclature.

with foods has been investigated: namely the 2,3-dibenzylbutanes, 2,3-dibenzylbutyrolactones, 2-aryl-4-benzyl-tetrahydrofurans, aryltetralins, and furofurans (Fig. 24). Sugars, if present, are removed by the gut microbiota and the aglycones are further transformed.

These aglycone transformation products are commonly referred to as enterolignans and include 2,3-dibenzyl-butan-1,4-diols, 2,3-dibenzyl-butyrolactones and 1,2-dibenzyl-cyclopentanes (for specimen structures see Fig. 25–27). The known substitution patterns of the aromatic moieties are 4′-hydroxy-3′,5′-dimethoxy-, 3′,4′-dimethoxy-, 4′-hydroxy-3′-methoxy-, 3′,4′-dihydroxy-, 3′,4′-methylenedioxy-, and 3′-hydroxy-(either benzyl or phenyl depending on the enterolignan class), and these occur in several combinations.[66–70] Structures are shown in Fig. 25–27 for the unconjugated metabolites. Note that for matairesinols, which do not possess C_2-symmetry, two regioisomers are possible if the aromatic substituents are different (Fig. 26).

Quartieri *et al.*[70] reported 25 enterolignan sulfate, glucuronide, and sulfo-glucuronide conjugates in human urine after volunteers consumed secoisolariciresinol-diglucoside and this is almost certainly an under-estimate because there was no allowance made for regioisomerism of either the aromatic moieties or for the phase-II conjugating moiety attached thereto. For example, it has previously been reported that human urine may contain two mono-glucuronides and two mono-sulfates of both enterodiol and enterolactone[71–73] but note that human phase-II metabolism of enterodiol and enterolactone is predominantly mono-glu-

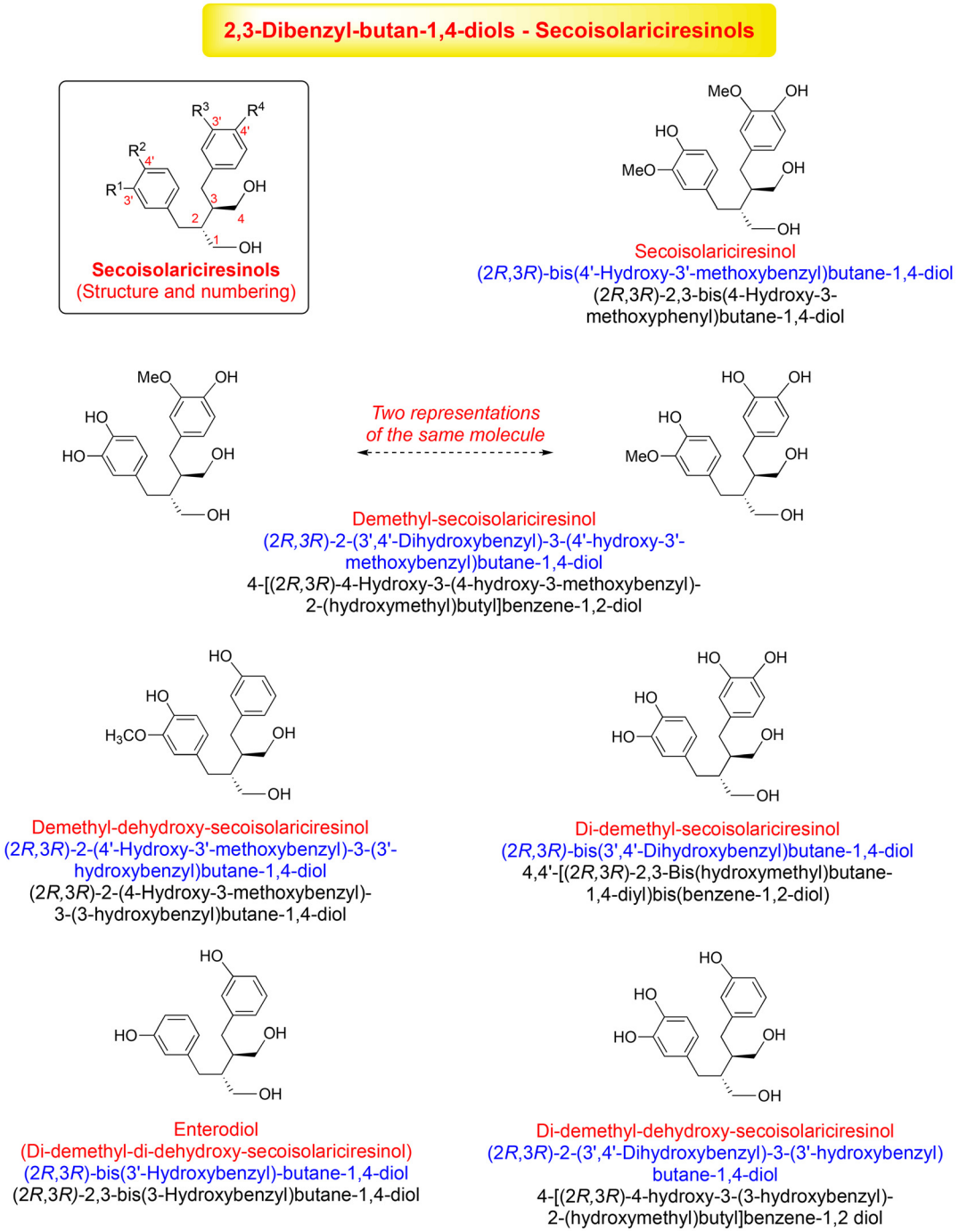

Fig. 25 Secoisolariciresinol and its associated gut microbiota catabolites. Red names – synonyms, blue – recommended nomenclature, black – IUPAC nomenclature.

curonidation with only a small contribution from monosulfates.

The IUPAC rules for naming these unconjugated enterolignans are complex and clumsy, and the approach adopted varies significantly depending on the class of metabolite (see names in black in Fig. 24–26). The literature contains numerous approaches, which do not allow easy comparison and meta-analysis, so we propose a system which is more uniform across the main classes of metabolites and consistent with our previous recommendations.[29] These proposals are straightforward for metabolites where both aromatic moieties are identical, less so for matairesinols when they are different, because there is no easy method for distinguishing the regioisomers.

As stated earlier, once the structure of a catabolite has been defined using the recommended nomenclature, it is acceptable to associate it with a trivial name, which is subsequently used in

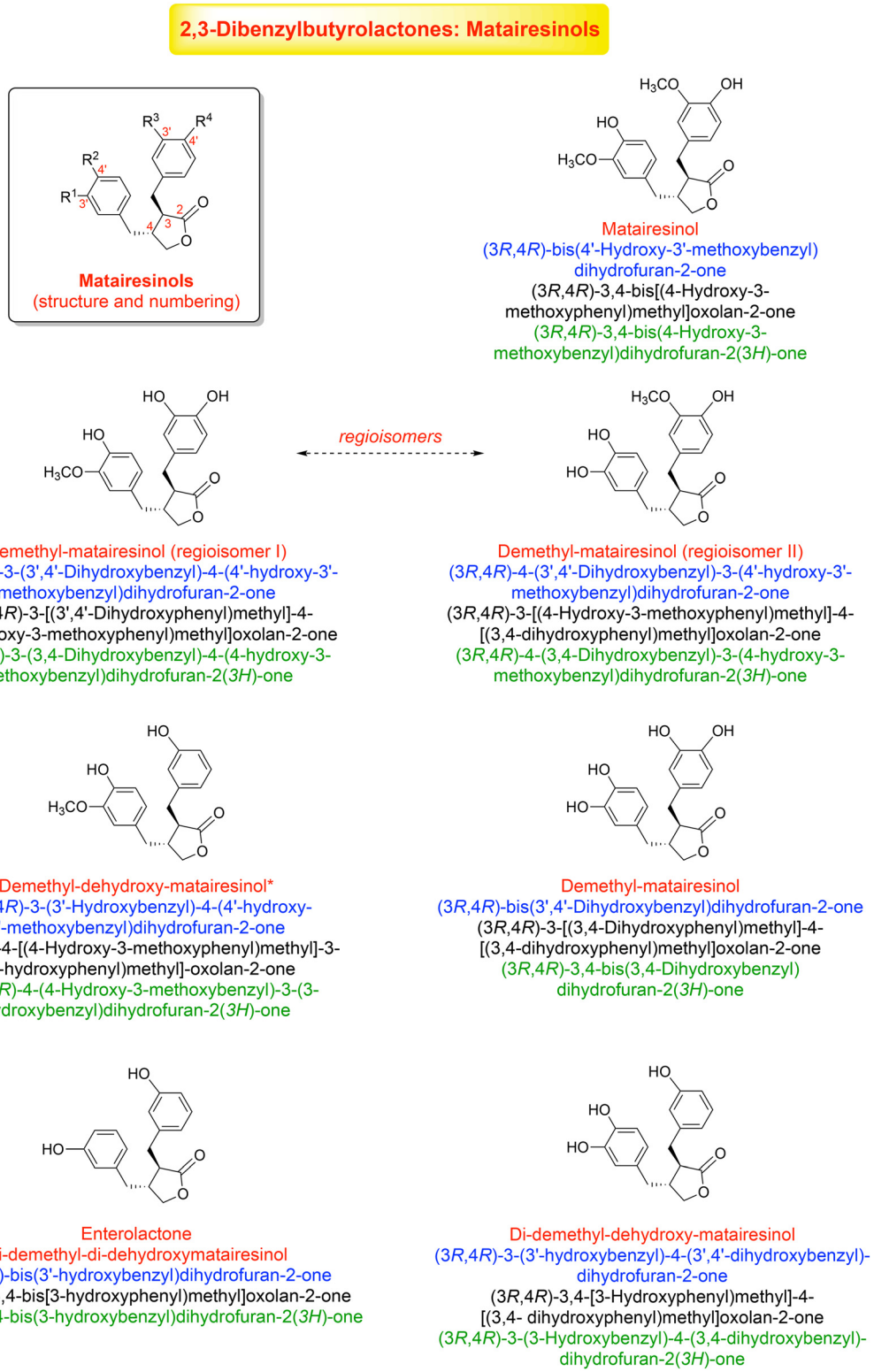

Fig. 26 Matairesinol and its associated gut microbiota catabolites. Red names – synonyms; blue – recommended nomenclature, black – IUPAC traditional, green – IUPAC nomenclature *via* Chemdraw. * – two possible regioisomers, only one shown.

the text. Relatively few of the enterolignans, however, have trivial names, but the approach used by Quartieri *et al.*[70] is convenient. This system of nomenclature utilizes the trivial name of the substrate and records how many demethylations and/or dehydroxylations have produced the metabolite. For example, the plant lignan secoisolariciresinol, for which we recommend (2*R*,3*R*)-bis

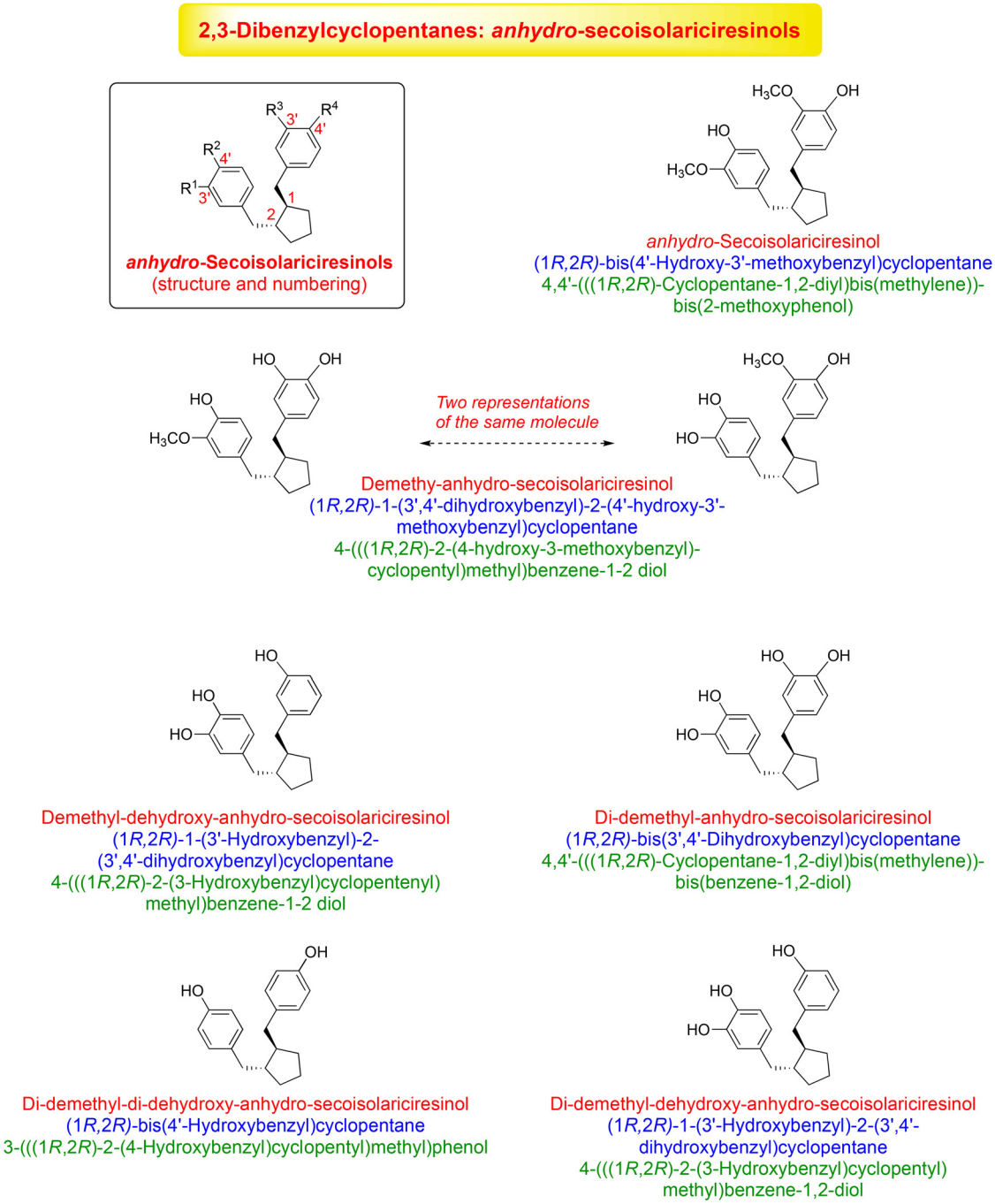

Fig. 27 Anhydro-secoisolariciresinol and its associated gut microbiota catabolites. Red names – synonym, blue – adjusted to simplify with inconsistencies removed to correspond as closely as possible to our existing recommendations, green – IUPAC nomenclature *via* Chemdraw.

(4′-hydroxy-3′-methoxybenzyl)butane-1,4-diol, is transformed by the gut microbiota yielding demethyl-, di-demethyl-, demethyl-dehydroxy-, di-demethyl-dehydroxy- and di-demethyl-di-dehydroxy-secoisolariciresinol as illustrated in Fig. 24. Fig. 26 and 27 provide the corresponding information for 2,3-dibenzyl-butyrolactones and 1,2-dibenzyl-cyclopentanes. This simplified nomenclature is particularly of interest when the positions where the demethylations and/or dehydroxylations take place are unknown.

Until such time as the phase-II conjugates are fully characterized and authentic standards are available, such conjugates should be described as "a sulfate/glucuronide/sulfo-glucuronide conjugate of secoisolariciresinol", *etc*. This does not help to improve the accuracy of databases like PhytoHub and HMDB, but it represents a conservative approach that may avoid further mistakes.

As discussed for other classes of metabolites, the vendors' literature is inconsistent. Some of the vendors listed on

Pubchem¶¶ and Chemspider‖‖ show an undefined enterolignan structure, and others show one enantiomer, but these structures are presented from a variety of perspectives. The naturally occurring C_2-symmetrical (−)-(2*R*,3*R*)-enantiomer of secoisolariciresinol, its antipode the (+)-(2*S*,3*S*)-enantiomer, and the racemic mixture are commercially available. The *meso*-form has been synthesized, and *in vitro* studies indicate that biological activity varies with the isomer tested.[74,75] Similarly, racemic and optically pure (2*R*,3*R*)-matairesinol are to be found in vendors' listings, but prospective purchasers should obtain written confirmation regarding enantiomeric purity if a specific isomer is required.

4. Conclusions

The relentless advances of metabolomic research continue to increase the number of metabolites reported, particularly those produced from dietary (poly)phenols by the microbiota, and which are thought to be responsible for some of the beneficial effects of a plant-based diet. These microbial metabolites constitute an extremely diverse set of polyfunctionalized chemical structures many of which have regioisomeric and stereoisomeric forms. Such isomers are likely to differ in their biological activity.

Recognition that such metabolites are inconsistently described in the literature and sometimes even overlooked, persuaded us to focus upon the stereoisomeric forms of chiral metabolites (enantiomers and diastereomers) and expand the proposals for the nomenclature of (poly)phenol metabolites made by Kay *et al.*[29] Our intention is to establish a convenient, clear, and unambiguous nomenclature in a modality to be read and understood also by non-chemists who often have difficulty in 'reading' 3-dimensional structures expressed in 2-dimensions. We believe that the use of this consistent and unambiguous nomenclature will facilitate data retrieval for meta-analysis and the preparation of critical systematic reviews, which ultimately will improve our understanding of the biological effects of these metabolites.

We also recommend that identifications and tentative identifications are categorized as Metabolomics Standards Initiative levels 1 or 2 according to Sumner *et al.*[76] Tentative level 2 identifications are made in the absence of authentic reference compounds and, consequently, quantitative data so obtained should be treated with caution and viewed only as estimates.

Abbreviations

CAS	Chemical Abstracts Service Registry Number (also referred to as CASRN)
C_{max}	Peak plasma concentration
InChIKey	IUPAC International Chemical Identifier
IUPAC	International Union of Pure and Applied Chemistry
L-DOPA	L-3′,4′-Dihydroxyphenylalanine

¶¶ https://pubchem.ncbi.nlm.nih.gov/compound/65373#section=Chemical-Vendors

‖‖ https://www.chemspider.com/Chemical-Structure.58845.html?rid=3fab6e1e-69d3-4563-99b4-c7cc30aeb390&page_num=0

Author contributions

C. C., M. N. C., C. D. K. and A. C. conceived the study, and wrote the first version of the manuscript, edited drafts and had responsibility for the final content. P. M., A. R.-M., D. D. R., G. W. and G. J. M. helped edit drafts of the manuscript. D. M. assisted with some of the figures. All authors: contributed to various versions the text and read and approved the final version of the manuscript.

Data availability

Data files are available on requested from Alan Crozier at alan.cozier44@gmail.com.

Conflicts of interest

The authors declare no conflicts of interest.

Acknowledgements

C. C. received financial support from the University of Parma. C. D. K. was funded by USDA-ARS project 6026-10700-001-000D. P. M. and D. D. R. were supported by the National Recovery and Resilience Plan of the Italian Ministry of University and Research funded by the European Union-NextGenerationEU; Award Number: PE00000003 "ON Foods – Research and innovation network on Food and Nutrition, Sustainability, Safety and Security – Working ON Foods". G. M. D. was supported by the Rural & Environment Science & Analytical Services Division of the Scottish Government" A. C., G. P.-C. and C. I. R. G. were funded by the Distinguished Scientist Fellowship Program (DSFP) of King Saud University, Riyadh, Saudi Arabia.

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