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## **EUROFIR WP1.8 TG2.2**

### **EUROFIR COMPONENT THESAURUS REPORT**

### **REPORT ON THE PREPARATION OF VERSION 1.2**

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#### **ABSTRACT:**

*The EuroFIR Component Thesaurus provides a list of authoritative codes and descriptors for identifying food components in data reporting the composition of foods. Version 1.0, published in 2008, was extensively revised in the release, version 1.1. Version 1.2 has now been prepared and this report documents the changes, together with background information collected during the revision process. Some outstanding issues will need further consideration before decisions are implemented in future versions, such as version 2.0 due at the end of 2010.*

*New terms were added and revisions made at the request of data compilers or to correspond to INFOODS tagnames. Extensive discussions with INFOODS, who have been updating their tagname list at the same time, have led to considerable harmonisation of the two thesauri, particularly with regard to organic acids and bioactive components. Where appropriate, specific INFOODS tagnames and eBASIS identifiers have been added to the Additional Information field in the Component Thesaurus. Scope notes for existing terms have been added or improved and extra synonyms were included.*

# EuroFIR component thesaurus report

## Report on the preparation of version 1.2

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## Introduction

This document records the changes made in preparing version 1.2 of the EuroFIR Component Thesaurus. The revisions are more targeted than the extensive editing that was undertaken to produce version 1.1 (Unwin, 2010). In particular it includes work to add further organic acids, to add bioactive components corresponding to those in the 2010 update to the INFOODS tagname list and to add extra INFOODS tagnames where a Component Thesaurus identifier relates to more than one more specific tagname. It also includes changes identified as necessary by ETHZ during their implementation of calculations in food database management software, ensuring that all components contributing to a Method Indicator Thesaurus calculation method are supported in the Component Thesaurus.

Editing is performed using the Thesaurus Manager software, which also permits read-only access by a wider audience of thesaurus users. This is now available on the EuroFIR server at:

<http://ethesaurus.eurofir.org/> (username: eThesaurusGuest, password: guest\$Welcome).

Since early 2009, all changes to the thesaurus have been documented in the Editor's notes field of Thesaurus Manager.

## Carbohydrate components

### *Polysaccharides*

The energy-contributing ingredient "polydextrose" [POLYDEXS] has been added to the Component Thesaurus as it contributes to the Method Indicator energy calculation MI0109. Polydextrose is a glucose polymer, being an ingredient synthesised from dextrose, about 10% sorbitol and 1% citric acid. Its e-number is E1200 and the synonym "polyglucose" has been included. As this is strictly an additive rather than a component (see section below on *Food additives*), the entry includes a scope note stating "Use to manage the composition in foods of this ingredient when this is required for energy calculation purposes".

## Lipid components

### *Fatty acids*

The component "fatty acid 24:1 trans" [F24:1TRS] was added, used for total trans-tetracosenoic acids, as this can contribute to summations of monounsaturated fatty acids, for example in the calculation method MI0211.

## Nitrogen components

### *Amino acids*

The Swiss database requested the term for "amino acids, total essential; eight essential amino acids" [AAE8], corresponding to the equivalent INFOODS tagname, and this was added. Also, an entry for "amino acid nitrogen" [AAN] was proposed as this is cited in the Method Indicator "Protein calculated from amino acid nitrogen" [MI0121]. Alternatively, the entry for this might be "nitrogen, amino acid" [NAA] to keep it consistent with NT and NNP ("total" and "non-protein", respectively). Primary amino acids (i.e. all the common amino acids except proline) can be determined analytically (Dukes and Butzke, 1998; Vintessential Laboratories, 2010), but alternative methods may include secondary amino acids. Some further investigation will be required to establish the methods for determining amino acid nitrogen that need to be documented using Method Indicator terms. The term "nitrogen, amino acid" [NAA] has been added for version 1.2, although this can be reviewed further in future updates.

## Organic acids

### Definition and hierarchy

Organic acids were discussed by the classic text (Merrill and Watt, 1955, pp 6-7), which reported their energy content on the basis of their “heats of combustion or gross caloric values per gram of acid calculated from gram-molecular weight data”. Neither this reference nor later documents such as the FAO report on food energy (FAO, 2003) and the EU Labelling Regulations (EEC, 1990; EC, 2003; EC, 2008; EP, 2008; EP, 2009) provide a definition of “organic acid”. IUPAC does not include “organic acid” in its glossary of class names<sup>1</sup> and it is not a MESH term in MEDLINE. In lieu of a more specific definition, fatty acids are organic acids, but it would not be sensible to include these, since these are constituent parts of the fat component and are considered separately. Thus a suitable working definition is required.

The Wikipedia definition<sup>2</sup> of an organic acid is an organic compound with acidic properties, which includes *inter alia* sulphonic acids as well as carboxylic acids. There are significant food components that are sulphonic acids, e.g. taurine (2-aminoethanesulfonic acid), but for nutritional purposes the definition might be limited to carboxylic acids. Both fatty acids and amino acids (whether free or in a combined state) must be excluded and there may be further classes of carboxylic acids that should not be included. However, the definition “An organic acid is any carboxylic acid, with one or more carboxyl groups, that is not a fatty acid or an amino acid” might serve as a suitable starting point. It is also necessary to define fatty acid, in particular the shortest chain alkanoic acid that is excluded from the organic acids group, which is presumably butanoic acid since this is normally counted as a fatty acid. This definition of organic acid excludes esters, lactones and acids where the hydrogen ion derives from a non-carboxylic functional group. This excludes, for example, ascorbic acid, but a further refinement is needed if compounds such as pantothenic acid are to fall outside the definition.

Organic acids are reported in food composition data for several reasons that may be relevant to their inclusion in the Component Thesaurus. As well as contributing to the calculation of energy, they may cause adverse reactions in humans, some are important for taste of foods and some act as natural or added preservatives. In some foods, the amount of organic acids present is sufficient to be required in the validation of a food composition record as totalling 100g per 100g of food.

In version 1.1, the term “organic acids, total” [OA] has the scope note “Use for total of energy-contributing organic acids only”, although this may not be useful as all organic acids make some contribution to energy. However, if the energy for a food includes a contribution using the general factor for organic acids, for example as reported by the Method Indicators MI0103 or MI0104, the identifier OA reports the organic acids total used in the calculation. Thus the scope note has been revised to read “Use for the total of organic acids, i.e. carboxylic acids that are not fatty acids or amino acids. Where the contribution to energy is calculated using a general factor for organic acids, the compositional value for total organic acids [OA] must be the value used in the energy calculation”. The EU Labelling Regulations and other guidelines specify the energy conversion factor for organic acids as 3 kcal/g or 13 kJ/g, but some applications may use specific conversion factors for individual acids. These may vary considerably, since logically that for benzoic acid will be much lower than that for acetic acid, for example. Information on any factors used in calculations for individual organic acids forms part of the method information for an energy value, although current specifications may need to be enhanced to accommodate this aspect of method documentation.

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<sup>1</sup> <http://www.chem.qmul.ac.uk/iupac/class/>, accessed 2010-05-18.

<sup>2</sup> [http://en.wikipedia.org/wiki/Organic\\_acid](http://en.wikipedia.org/wiki/Organic_acid), accessed 2010-05-04.

### Individual organic acids

The Danish component list includes formic, acetic, propionic, lactic, citric and isocitric acids expressed in grams, together with oxalic, malic, succinic, chinonic (quinonic), tartaric, benzoic, salicylic, sorbic and adipic acids expressed in milligrams. These were all covered in the original Component Thesaurus except for quinonic acid and adipic acid (1,6-hexanedioic acid). In the version 1.1 work, quinonic acid was considered to be quinolic acid (pyridine-2,3-dicarboxylic acid). The two components were added in version 1.1 using the more common descriptor “quinolinic acid” for the pyridine derivative (with “quinolic acid” as a synonym) and the codes QUINLAC and ADIAC.

The Merrill and Watt report also lists glyoxalic acid (which has the synonyms glyoxylic acid, oxoacetic acid and formylformaldehyde), aconitic acid (which has various synonyms, including prop-1-ene-1,2,3-tricarboxylic acid and citridinic acid, sometimes relating specifically to the *cis* isomer) and malonic acid (propanedioic acid).

The following table lists the organic acids in the Component Thesaurus version 1.1 and those considered as new entries in version 1.2. The main sources that have been checked for possible organic acids to be included are the INFOODS tagnames list (✓) including recent updates (2008 and 2010), the Danish data and the original paper on the energy values of foods noted above (Merrill and Watt, 1955).

Identifier	Descriptor	EuroFIR	INFOODS	DK	Notes
ACEAC	acetic acid	✓	✓	✓	Synonym: ethanoic acid
ADIAC	adipic acid	✓		✓	Synonym: 1,6-hexanedioic acid
ACONAC	aconitic acid	added		✓	Merrill & Watt. Synonyms: prop-1-ene-1,2,3-tricarboxylic acid, citridinic acid, etc. Sometimes specifically the <i>cis</i> or <i>trans</i> isomer. ACONAC was assigned as a new code
BENAC	benzoic acid	✓	✓	✓	Synonym: dracrylic acid, phenyl-carboxylic acid, phenylformic acid, E210
CHLRAC	chlorogenic acid	added	✓		Synonyms: 3-caffeoylquinic acid, 3-(3,4-dihydroxycinnamoyl)quinic acid. Probably should also be grouped as a phenol or tannin
CITAC	citric acid	✓	✓	✓	Synonym: 2-hydroxypropane- 1,2,3-tricarboxylic acid
FERAC	ferulic acid	added	✓		Synonyms: 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid, 3-methoxy-4-hydroxycinnamic acid
FORAC	formic acid	added	✓	✓	Synonym: methanoic acid
FUMAC	fumaric acid	✓	✓		Synonyms: trans-butenedioic acid, boletic acid, lichenic acid. The <i>cis</i> form (maleic acid) does not occur naturally.
GALAAC	galacturonic acid	added	✓		Synonym: (2S,3R,4S,5R)-2,3,4,5-tetrahydroxy-6-oxo-hexanoic acid
GALLAC	gallic acid	added	✓		Synonym: 3,4,5-trihydroxybenzoic acid

Identifier	Descriptor	EuroFIR	INFOODS	DK	Notes
GLYCLAC	glycolic acid	added	✓		Synonyms: hydroxyacetic acid, 2-hydroxyethanoic acid
GLYOXAC	glyoxalic acid	added			Merrill & Watt. Synonyms: glyoxylic acid, oxoacetic acid, formyl-formaldehyde. GLYOXAC was assigned as a new code
GLUAKAC	alpha-keto-glutaric acid	added	✓		Synonym: 2-oxopentanedioic acid
GLUCAC	gluconic acid	added	✓		Added as D-gluconic acid, although the INFOODS descriptor does not specify the stereoisomerism. Synonym for D-gluconic acid: dextronic acid
ISOCAC	isocitric acid	✓	✓	✓	Synonym: 1-hydroxypropane-1,2,3-tricarboxylic acid
LACAC	lactic acid	✓	✓	✓	Synonym: 2-hydroxypropanoic acid
LACACD	D-lactic acid	✓	✓		
LACACL	L-lactic acid	✓	✓		
MALAC	malic acid	✓	✓	✓	Synonym: hydroxybutanedioic acid. L-Malic acid is the naturally occurring form.
MALONAC	malonic acid	added	✓	✓	Merrill & Watt. Code agreed with INFOODS as MALONAC. Synonym: propanedioic acid
OA	organic acids, total	✓	✓		Scope note discussed in text, above.
OXACAC	oxaloacetic acid	added	✓		Synonyms: oxosuccinic acid, oxobutanedioic acid
OXALAC	oxalic acid	✓	✓	✓	Synonym: ethanedioic acid
PARHBAC	para-hydroxybenzoic acid	renamed	✓		Renamed from parahydrobenzoic acid.
PHYTAC	phytic acid	✓	✓		Not strictly an organic acid since the acid moieties are phosphate groups. Synonym: inositol hexaphosphate.
PROPAC	propionic acid	✓	✓	✓	Highest alkanolic acid that is not a fatty acid
PYRAC	pyruvic acid	added	✓		Synonyms: 2-oxopropanoic acid, $\alpha$ -ketopropionic acid, acetylformic acid, pyroracemic acid
PYROGAC	pyroglutamic acid	added		✓	Synonyms: pidolic acid, 5-oxo-L-proline. Lactam from glutamic acid, retaining L configuration. PYROGAC was assigned as a new code

Identifier	Descriptor	EuroFIR	INFOODS	DK	Notes
QUINAC	quinic acid	✓	✓		Synonyms: (1S,3R,4S,5R)-1,3,4,5-tetrahydroxycyclohexanecarboxylic acid, chinic acid. Possibly should be listed as a phenolic compound or tannin rather than as (or as well as) an organic acid.
QUINLAC	quinolinic acid	✓		✓	Synonyms: pyridine-2,3-dicarboxylic acid, quinolic acid
SALAC	salicylic acid	✓	✓	✓	Synonym: 2-hydroxybenzoic acid
SHIKAC	shikimic acid	<b>added</b>	✓		Synonym: (3R,4S,5R)-3,4,5-trihydroxycyclohex-1-ene-1-carboxylic acid
SORAC	sorbic acid	✓		✓	Synonym: 2,4-hexadienoic acid
SUCAC	succinic acid	✓	✓	✓	Synonym: butanedioic acid
TARAC	tartaric acid	✓	✓	✓	Synonym: 2,3-dihydroxybutanedioic acid, 2,3-dihydroxysuccinic acid, threarc acid, uvic acid. The naturally occurring form is L-tartaric acid.
GRP_STERAC	Steroid acids				Group removed
GULDKAC	diketogulonic acid	<b>renamed</b>			Renamed from “di-keto-cholanic acid”, with scope note “Use for (4R,5S)-4,5,6-trihydroxy-2,3-dioxohexanoic acid (2,3-diketo-L-gulonic acid), the degradation product of dehydroascorbic acid”. No entry was created for the possible component “di-keto-cholanic acid” (see section below)

The above list indicates organic acids that were added or revised for version 1.2. The additions are aconitic acid [ACONAC], formic acid [FORAC], malonic acid [MALONAC] and para-hydroxybenzoic acid [PARHBAC]. The descriptor for GULDKAC was revised to “diketogulonic acid” as this seems the most appropriate component resulting from the investigation of possible meanings, recorded in the section below.

The added organic acids mostly corresponding to existing INFOODS tagnames or are included in the Merrill & Watt paper. These are chlorogenic acid [CHLRAC], ferulic acid [FERAC], galacturonic acid [GALAAC], gallic acid [GALLAC], glycolic acid [GLYCLAC], glyoxalic acid [GLYOXAC], alpha-keto-glutaric acid [GLUAKAC], gluconic acid [GLUCAC], oxaloacetic acid [OXACAC], pyruvic acid [PYRAC] and shikimic acid [SHIKAC]. New or revised identifiers are mentioned in the Notes column.

### Synonyms

The above table gives various synonyms for individual organic acids. The alphabetical listing of the thesaurus is the main way that a user will access terms through a synonym and thus it is not useful to include synonyms that start with locants or other indicators of minor structural variation. The policy to be followed for the organic acids, in line with other groups of components, is to include only trivial names and useful systematic names as full synonyms, but to include definitive systematic names and any important but alphabetically unhelpful synonyms in the scope notes for the component. For example, for “tartaric acid” [TARAC], “uvic acid” is included



as a synonym and the scope note reads “Use for L-tartaric acid, i.e. (2R,3R)-2,3-dihydroxybutanedioic acid”.

### ***GULDKAC, di-keto-cholanic acid?***

Inversion 1.1 and earlier lists, this entry had the anomalous code GULDKAC, which may indicate an unspecified synonym. Otherwise, there is no information on the intended compound(s). Investigation found that cholanic acid is ChEBI 36237 and cholic acid (ChEBI 16359) is its 3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -trihydroxy derivative. Some reference was found to 3,6-diketocholanic acid, which is structurally similar to the bile acid chenodeoxycholic acid (3 $\alpha$ ,7 $\alpha$ -dihydroxy-5 $\beta$ -cholan-24-oic acid) apart from the position of the second keto/hydroxy group. Hyodeoxycholic acid (ChEBI 52023) is 3 $\alpha$ ,6 $\alpha$ -dihydroxy-5 $\beta$ -cholan-24-oic acid and thus is the tetrahydro analogue of 3,6-diketocholanic acid.

Considering the code (and ignoring the name), it is possible that GULDKAC represents 2,3-diketogulonic acid. This has the formula  $\text{CH}_2(\text{OH})\text{CH}(\text{OH})\text{CH}(\text{OH})(\text{CO})_2\text{CO}_2\text{H}$  and is the inactive product arising when the lactone ring of dehydroascorbic acid is irreversibly opened. This is perhaps the most likely source of the term as it relates to a known food component (Matthews and Hall, 1978). Therefore, the descriptor for GULDKAC has been revised to “diketogulonic acid”, making it a valid component identifier. At present, no component based on a cholanic acid structure has been added.

### ***Phytic acid***

Following the approach taken in the Eurofoods Recommendations thesaurus, PHYTAC was classified as an organic acid, although it is a phosphoric acid derivative. It can also be considered an inositol derivative, i.e. an inositol with phosphorylated hydroxyl groups. On this basis, PHYTAC has been copied to the *Sugar alcohols* group. Within the organic acids group, a sub-group such as “phosphoric acid derivatives” might be an informative aid to users, particularly with the addition of the inositol phosphoric acids described below. The previous Additional Information text “The placing of PHYTAC under Organic acids is probably not correct, but no better place has been identified in the present component hierarchy” has been revised to “Phytic acid is a phosphate derivative of a polyol. In the present component hierarchy, PHYTAC is placed in both the Sugar alcohols and Organic acids sections for clarity, although it does not conform to the strict definition of an organic acid as a carboxylic acid”.

The Swiss database has a requirement for additional inositol phosphate components, namely inositol monophosphate (IP1), inositol diphosphate (IP2), inositol triphosphate (IP3), inositol tetraphosphate (IP4) and inositol pentaphosphate (IP5). These components were added, using the identifiers INOTLP $n$ , where  $n = 1$  to 5, with PHYTAC remaining the code for IP6 (phytic acid). No isomeric detail was included in the definitions, although ChEBI has separate entries for several isomers for the diphosphate upwards. These are recorded in the Additional Information field. Only IP6 and IP5 seem to reduce bioavailability of certain other compounds, although the lower phosphorylated forms may act as anticarcinogens. The official AOAC method for phytic acid seems to overestimate true IP6 content as it measures total P of all inositol phosphates (Lehrfeld and Morris, 1992).

### **Bioactive components**

It was agreed that the full set of eBASIS bioactive components would not be added to the Component Thesaurus at this stage. However, the 38 components from the original COST listing of “Bioactive constituents” have been included in existing versions of the EuroFIR thesaurus, with identifiers harmonised with INFOODS tagnames. They are well-known constituents with simple trivial names. The latest list of candidate INFOODS tagnames includes further bioactive substances with simple trivial names and this limited range of bioactive components has been added to the Component Thesaurus to maintain commonality with the tagnames list.

Extra or revised components in version 1.2 are:

Identifier	Descriptor	eBASIS	ChEBI	Notes
ADEN	adenine	1320	16708	6-aminopurine
ANTCYAN	anthocyanidins, total			Included in the INFOODS 2010 proposals, limited to the free forms and excluding glycosides. This contrasts with eBASIS 1928, which is “Total anthocyanins”, which must cover the glycosides, although it is uncertain whether this includes the anthocyanidin aglycones.
APIGEN	apigenin	1439	18388	In version 1.1, moved to Flavones
CAPSA	capsaicin	21	3374	trans-8-methyl-N-vanillyl-6-nonenamide
CATEC	(+)-catechin	1420	15600	In version 1.1 as “catechin”, changed to common stereoisomer and moved to Flavanols.
CATECT	catechins, total	1736		Included in the INFOODS 2010 proposals. A definition will be needed, which may include gallic catechins, catechin gallates, or all flavan-3-ols
CYAD	cyanidin	1549	27843	
DELPH	delphinidin	1552	28436	
EPICATEC	epicatechin	1417	28466	In version 1.1, moved to Flavanols. (-)-epicatechin, ChEBI added
EPICATECG3	epicatechin-3-gallate	1423		
EPICATEGC	epigallocatechin	1424	42255	
GALCATEGC	gallic catechin	1427		
HESPD	hesperidin	1432	28775	
HESPT	hesperetin	1431	28230	
KAEMF	kaempferol	1483	28499	In version 1.1, moved to Flavonols. ChEBI added
LUTEOL	luteolin	1458	15864	In version 1.1, moved to Flavones, ChEBI added
MALVIDIN	malvidin	1565		
MYRIC	myricetin	1506	18152	In version 1.1, moved to Flavonols. ChEBI added
NARIN	naringin	1999	28819	
NARING	naringenin	1985	50202	
NARIR	naringin	2096	28705	INFOODS: “A flavanoid comprised of the flavanone naringenin and the disaccharide rutinose”

Identifier	Descriptor	eBASIS	ChEBI	Notes
PEONIDIN	peonidin	2014		
PETUNIDIN	petunidin	1582		
PROCYA	procyanidins, total			Proanthocyanidin and procyanidin are synonyms used for polymers (from dimers up) of flavan-3-ols. eBASIS: has "Proanthocyanidin Total" = 1863; "Procyanidin" = 1837, although the difference is not clear.
QUERCE	quercetin	1509	16243	In version 1.1, moved to Flavonols. ChEBI added
RUTIN	rutin	2013	28527	INFOODS: "A quercetin-3-rutinoside; rhamno-(1-6)-glucoside of quercetin". eBASIS: "Quercetin-3-rutinoside" = 1526; possibly a duplicate
TANGER	tangeretin	2012	9400	

eBASIS identifiers have been added to the Additional Information field of the thesaurus entry, both for the existing and new bioactive components. As well as phenolic components, these included carotenoids, phytosterols and cinnamic acid derivatives.

### ***Phenolic components hierarchy***

A more formal hierarchy has been applied to the *Phenolic components* group. New sub-groups for *Capsaicinoids* and *Flavonoids* have been added alongside the existing *Phytoestrogens* group. The *Flavonoids* group has been subdivided into *Anthocyanidins* and *anthocyanins*, *Flavanols*, *Flavanones*, *Flavones* and *Flavonols*. The sub-groups *Isoflavonoids* and *Lignans* have been added under the *Phytoestrogens* group. The structures in each group have been described in the Additional Information field of the group terms.

## **Vitamins and related compounds**

### ***Carotenoids***

The identifier for "capsanthin" was changed from CAPSA to CAPSCIN in version 1.1 to harmonise with the INFOODS tagname. However, it has been noted that the identifier/tagname CAPSCIN mixes the names of "capsanthin" (which has no second "c") with "capsaicin", which appears in the above list of bioactives and is represented by CAPSA in the current INFOODS proposals for new tagnames. Therefore, the alternative identifier of CAPSAN for "capsanthin" has been used and proposed to INFOODS. Inverted names such as "carotene, alpha-" have been added as synonyms to aid the location of carotenoids in the alphabetical listing of descriptors. Also, IUPAC carotenoid names have been added to the scope notes to aid recognition when comparing information with other sources.

### ***Niacin***

At present, niacin can only be reported as a total of nicotinic acid and nicotinamide. However, in the calculation of NIAEQ as "Niacin equivalents calculated from niacin and tryptophan" [MI0421], the value for niacin may be derived from separate values for nicotinic acid and nicotinamide. Thus these contributing components have been added to the Thesaurus, using the codes

NICOTAC for nicotinic acid and NICOTAM for nicotinamide. A Method Indicator may be required for the summation  $NIA = NICOTAC + NICOTAM$ .

In reviewing the MI0421 calculation of NIAEQ as  $NIA + TRP/60$ , it has also been suggested that the activity unit *niacin equivalent* should be defined in the Component Thesaurus scope note as “1 Niacin equivalent = 1 mg Niacin”. The unit NE, “niacin equivalent”, appears in the current version of the EuroFIR Unit Thesaurus, without further definition. A carefully constructed definition is needed that takes account of the variable bioavailability of niacin. The alternative calculation, MI0422, gives NIAEQ as  $NIA \times 0.3 + TRP/60$ , i.e. “1 Niacin equivalent = 3.3 mg Niacin”. Thus the definition needs some further qualification, for example as “1 Niacin equivalent = 1 mg free Niacin” or “1 Niacin equivalent = 1 mg Nicotinamide”. A rigorous definition should be formulated.

### **Folates**

The scope note for “folate, total” [FOL] was extended to read “Use for total folate, including the contributions of both intrinsic food folate and synthetic folic acid” and the further Additional Information text “Total folate includes intrinsic food folate (FOLFD) plus the contribution of any synthetic folic acid (FOLAC) present. The calculation method is documented using the appropriate Method Indicator identifier.” has been added.

### **Food additives**

At present, components that are food additives have only been grouped under the *Food additives* heading if they do not appear elsewhere in the classification, e.g. beta-carotene under *Carotenoids*. A number of components may be considered to belong to the *Food additives* heading, but a policy on this is needed before further components are linked to it. European and other legislation on additives specify the material that may be added to a food as an ingredient, whereas the Component Thesaurus contains identifiers for substances as they are analysed or otherwise reported in foods. Additives may be mixtures, salts or other substances that lose their discrete identity when they become a constituent part of a food. It is the resultant components within the food that are represented by the Component Thesaurus entities. For example, the ingredient thiamin nitrate is a permitted additive, but the reported component is thiamin, expressed as thiamin monochloride. Before further additives are added to the Thesaurus or the *Food additives* group is edited, policies regarding additives should be agreed, and thus such revisions will be considered for a future update, possibly version 2.0.

### **INFOODS tagname additions**

Version 1.1 of the Component Thesaurus reports in the Additional Information field a single INFOODS tagname for any given EuroFIR component identifier. However, tagnames are more specific than EuroFIR identifiers, since they also report the method where different analytical methods give non-comparable results. Multiple tagnames are also defined where the mode of expression differs, for example for sugars expressed as monosaccharide equivalents. Thus more than one tagname may be relevant to a EuroFIR identifier, which reports only the component itself. It was agreed that all the tagnames related to an entry in the Component Thesaurus should be included in version 1.2.

The form in which multiple tagnames would appear was considered. The single tagnames present in version 1.1 were placed in a subfield of the Additional Information, e.g. for vitamin B12 the text is “<INFOODS>VITB12”. Vitamin B6 provides a related example, but with multiple tagnames. The following three options were considered for reporting these under Additional Information.

#### **Option 1**

<INFOODS>VITB6A, VITB6C, VITB6-

## Option 2

<INFOODS>VITB6A (vitamin A total, determined by analysis), VITB6C (vitamin A total, determined by summation), VITB6- (vitamin A total, method of determination unknown)

## Option 3

<INFOODS>VITB6A (vitamin A total, determined by analysis)

<INFOODS>VITB6C (vitamin A total, determined by summation)

<INFOODS>VITB6- (vitamin A total, method of determination unknown)

Feedback favoured the latter two options, with option 3 providing useful additional information. Although the inclusion of end-tags would make the content more like formal XML, this was considered to be an unnecessary complication to editing and exporting the thesaurus information. Current INFOODS tagnames were added in format option 3, but it will be necessary to monitor further revisions to the tagname list to keep the Component Thesaurus information up-to-date.

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