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COMPONENT AND METHOD INDICATOR THESAURI, VERSION 1.1

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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, has been extensively revised in the new release, version 1.1. This report documents the changes, together with the reasons and policies behind them. It also identifies outstanding issues that need further consideration before decisions are implemented in future versions, including version 1.2 at the end of May 2010 and version 2.0 at the end of 2010.

The flat listing of terms in version 1.0 was upgraded to a polyhierarchical organisation, with each term linked to one or more broader terms. New terms were added at the request of data compilers or to meet other requirements and a few obsolete terms were made inactive. Some identification codes were modified to harmonise with INFOODS tagnames or to conform to consistent policies. Scope notes for existing terms were added or improved and extra synonyms were included. Policies for identifying mixtures and condensation products are proposed.

Some groups of components have been reviewed in depth. The identification of unsaturated fatty acids has been improved through the development of consistent policies for the representation of isomeric variations. The requirements for various vitamins have been investigated, in particular folates, carotenoids and retinoids. Developments in the reporting of vitamers and the calculation of vitamin activities will require further enhancements to both the Component Thesaurus and the calculation factors recorded through the Method Indicator Thesaurus.

Component and Method Indicator Thesauri, version 1.1

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Introduction

This report records the changes made to the original version 1.0 of the EuroFIR Component Thesaurus (Møller *et al.*, 2008) during the extensive editing undertaken to produce version 1.1. It also notes issues that remain to be decided, together with further editing, decisions or discussion that are required as a result of discussions with INFOODS to harmonise with the tagname system[1]. Some further revisions are planned for version 1.2, due at the end of May 2010, but other issues need extensive discussion and will be resolved for version 2.0, which is scheduled for release by EuroFIR AISBL at the end of 2010.

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

http://www.polytec.dk/eThesaurus/ (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. This information is only visible in the edit-enabled version of Thesaurus Manager and is not copied to newer versions of the thesaurus. It can be viewed in the XML output format of version 1.1.

General changes from version 1.0

Hierarchical organisation

The version 1.0 thesaurus was a flat list of component identifiers without any grouping of terms according to type of component. However, Thesaurus Manager supports the hierarchical organisation of terms in a flexible way that allows a term to be linked to more than one immediate parent (i.e. broader) term to create a so-called polyhierarchy. This facility has been used for a few groups of components, for example individual carotenoids are linked to the two broader terms *Vitamin A and related components* (under *Vitamins*) and *Lipid components*.

Some broad terms are not for use in identifying the component associated with values in compositional data. However, such terms may be useful for indexing in other contexts, for example as terms assigned to primary literature such as journal articles. The codes for all such terms are suffixed with the characters "_GRP" and have the scope note "This term is for CLASSIFICATION ONLY; DO NOT USE term to identify a specific component. Use a more precise narrower term".

Synonyms

In version 1.0, synonyms were included in parentheses in the descriptor, e.g. "fatty acid 10:0 (capric acid)". In these cases, the parenthetic name has been added as a synonym in the thesaurus entry, but generally the existing descriptor also retains the parenthetic synonym.

The alphabetical listing of the thesaurus is the main way that a user will access terms through a synonym and thus is not useful to include synonyms that start with locants or other indicators of minor structural variation. The general has been 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 "fatty acid 16:1 n-7 trans" [F16:1TN7], "palmitelaidic acid" is included as a synonym and the scope note reads "Use for palmitelaidic acid (trans-9-hexadecenoic acid)".

[1] http://www.fao.org/infoods/tagnames_en.stm

Additional information (AI)

If a component is in ChEBI[2], but does not have an INFOODS tagname, the second line of AI has been added as "<INFOODS>-" as the ChEBI identifier needs to be followed by "<INFOODS>" to work correctly.

Mixtures

Reported components may be mixtures either because their constituent components were not resolved during analysis or because the constituent components are aggregated into a single value. Where the result represents the total for a group of components, this will normally be defined as a separate descriptor term in the thesaurus, e.g. "total saturated fatty acids" [FASAT]. However, for mixtures of more arbitrary sets of components, the composite component will be represented as the constituent components linked by the plus sign. For example, the unresolved mixture "lutein plus zeaxanthine" is identified as LUTN+ZEA and the sum of a selection of cis monounsaturated fatty acids as F14:1CIS+F16:1CIS+F18:1CIS. As indicated in the section on *Vitamins and related compounds*, the previous code for "lutein plus zeaxanthine" [LUTEZEAX] is now deprecated.

The proposed format uses the plus sign without surrounding spaces, i.e. "A+B", not "A + B". However, this does give rise to a possible conflict with proposed future codes representing metal oxidation states, e.g. for "molybdenum 4+" [MO4+] and "nickel 2+" [NI2+]. Further discussion of possible conflicts in the use of the plus sign is needed. Although oxidation state will normally be defined through a terminal plus sign, on rare occasions both conventions might be used, e.g. FE2++FE3+.

Condensation products

Another general type of food component can be viewed as a condensation product. A condensation reaction is a reaction in which two moieties combine to form one single molecule, accompanied by the loss of a small molecule, often water. Food components that can be considered as condensation products include esters, other glycerides and higher sugars. Some condensation products that are reported as food components consist of the linking of members from two (or more) types of simpler component already represented in the thesaurus. For example, several retinyl esters have been requested as various combinations of a retinol stereoisomer with a fatty or other organic acid. Requiring separate entries when data are reported may form a considerable burden for thesaurus maintenance.

An alternative would be to allow the combination of descriptors for condensation products in a similar way to that described above for mixtures. Above, X+Y was defined to represent "and" for mixtures and analogously a symbol might be defined that represents the expression "combined with". Possibly this could be a pair of parentheses, i.e. (). The double character would introduce further possibilities. For example, it could enclose coding to specify further information about the combination such as whether an acyl group was linked to an oxygen or nitrogen atom, i.e. X(O)Y or X(N)Y. This approach might provide useful extra flexibility in reporting components without necessarily having to add a large number of new terms to the thesaurus.

In the case of retinyl esters, terms for all-trans-retinyl palmitate, all-trans-retinyl oleate, all-trans-retinyl stearate, all-trans-retinyl linoleate and all-trans-retinyl acetate have been requested. However, it is possible that the reason the palmitate, oleate, stearate and linoleate esters were analysed and reported was that they were the commonest fatty acids, rather than the only ones. To avoid the need to predefine identifiers for retinyl esters, and possibly to avoid the need to add them to the thesaurus at all, the esters could be represented by, for example, the identifier RETOL()F16:0 for retinyl palmitate. This approach would also be clearer and avoid any

[2] http://www.ebi.ac.uk/chebi/

problems of ambiguity in a code such as RETOLLIN. It should be discussed for introduction when version 2.0 is implemented.

Component grouping hierarchy

Some comment was received on the grouping for version 1.1. However, further feedback would be useful so that any possible improvements can be identified and applied in future revisions such as versions 1.2 and 2.0.

Proximates

Feedback indicated that the term *Proximates* is not generally useful as a component grouping, although no alternative suggestions were made. Main nutrients such as total protein need to be grouped together, even if they are linked elsewhere lower in the polyhierarchy, e.g. under *Nitrogen components*. Others such as energy, water and alcohol do not belong to any existing grouping. A possible solution would be to change *Proximates* to *Energy and major nutrients* (although this title does not perhaps strictly apply to water and ash). Otherwise, possibly *Macronutrients* is the best term in current usage, with *Macro components* as an alternative that might be useful within the Thesaurus without wider implications. This should be reviewed for version 2.0.

Sugars and polyols

It has been noted that in various contexts, polyols are distinct from sugars and should not be a narrow term under *Sugars*. Therefore, a new heading will be created at the same level for the polyol components. The group term *Sugar alcohols* is used as this is more descriptive and will sort adjacent to *Sugars* in the hierarchical listing, but this should be further reviewed for version 2.0. See also the later section on *Polyols*.

Fatty acids

It has been suggested that classification terms are required at the level of the general identifiers for individual fatty acids Fxx:yy (e.g. F18:1). It is proposed to create new classification codes following the convention of starting these with “GRP_”, e.g. “GRP_F18:1”. This would allow the existing codes, such as F18:1, to retain their current usage for values for total or unspecified isomers. It is considered necessary to introduce this in version 2.0 of the thesaurus, but it needs to be decided if this should only apply to monounsaturated fatty acids or also to polyunsaturated fatty acids. It is probably not helpful to do this for saturated fatty acids where the only variants are branched chain isomers.

Carotenoids

In an earlier draft grouping, both vitamin A active and inactive carotenoids were listed within the main group of *Lipid components*, but only the vitamin A active carotenoids were listed under *Vitamin A components*. The current hierarchies were:

Lipid components
Carotenoids
Carotenoids, vitamin A active
alpha-carotene*, etc.*
Carotenoids, vitamin A inactive
canthaxanthin*, etc.*

and:

Vitamins

Fat soluble vitamins

Vitamin A components

13-cis retinol*, etc.*

alpha-carotene*, etc.*

This approach was taken in order to use the hierarchical classification to group together components with similar properties and separate dissimilar components, and to use the polyhierarchical capability to do this in relation to more than one property, in this case fat solubility and vitamin activity. It might be argued that within the Lipid category, the vitamin A aspect should be ignored completely, although it was included as an aid to users by explicitly listing the inactive components.

However, some preference was expressed for either a single list of carotenoids or a full list in both places, on the grounds of usability and to avoid issues relating to the physiological aspect of the Vitamin A activity. Therefore, all carotenoids have now been grouped under a classification term *Carotenoids*, linked to both *Vitamin A components* and *Lipid components* as its broad terms, with the former of these renamed *Vitamin A and related components*. Using this approach, any activity measure (particularly beta-carotene equivalents) would be better placed directly under *Vitamin A components* rather than under *Carotenoids*. Now that a number of extra individual retinoids have been added to the thesaurus, an analogous group has been created for *Retinoids*, also linked to both *Vitamin A and related components* and *Lipid components* as parents.

This revision of the carotenoids hierarchy indicated some omissions and inconsistencies in the Thesaurus Manager software. At present, it appears not to be possible to reduce the number of parents for each individual carotenoid from two to one. Also, redundant groups such as *Carotenoids, vitamin A active* could not be deleted. When the entry for “carotenoids, total” was moved into the *Carotenoids* group within *Vitamin A and related components*, it did not automatically appear in the *Carotenoids* listing under *Lipid components*. It will be difficult to ensure during editing that all necessary polyhierarchical links are copied or moved correctly, in part because there is no indication at an entry that it (or a higher level) has multiple parents.

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 need to be linked under the *Food additives* heading, but a policy on this is needed. That the component is permitted under European legislation seems a suitable basis. However, before this editing is undertaken, it would be best to agree any further policies regarding additives. These are discussed further in the later section on *Food additives*.

Major nutrients

Energy

The original descriptors for ENERA and ENERC were “energy, gross, determined by direct analysis” and “energy, total metabolisable; calculated from energy-producing food components”, respectively. These have been edited to “energy, gross” and “energy, total metabolisable” to remove the reference to method. The scope notes have been expanded to specify the usage.

Protein

The existing EuroFIR scope note for “protein, total” [PROT] of “Protein calculated from a nitrogen value” contravenes the EuroFIR policy of component definitions being independent of

method. The identifier might also be used where a value has been derived by the summation of amino acids. Comments on the proposed scope note "Use for total protein determined by any method, such as calculation from nitrogen or by summation of amino acids" suggested that this might not mention method at all. The scope note has been revised to "Use for total protein" and the sentence "The method used to obtain a PROT value should be reported through Method Indicator and Method Parameter documentation." has been added to the Additional Information text.

Carbohydrate components

Available carbohydrate

Currently the EuroFIR identifier for "available carbohydrate" will remain as CHO, although EuroFIR may change it in the future to CHOAVL if this is seen to be advantageous for harmonisation. An alternative option would be to use CHOA or CHOG (Available or Glycaemic), making the difference explicit in a compatible way with the identifier/tagname for "total carbohydrate" [CHOT]. However, current feedback suggests that this might be considered a retrograde step.

This conclusion was partly based on problems with the term "available carbohydrate", as used in the scope note. Alternatives of "utilisable carbohydrate" and "digestible carbohydrate" were proposed. The latter might be preferred, since this more strongly implies human digestion rather than utilisable results of bacterial digestion (although this contrasts with the EU Labelling Directive, which uses the definition of "metabolized **in** man" rather than "metabolized **by** man"). Therefore, the scope note of "carbohydrate" [CHO] has been changed to "Use for total carbohydrates digested and absorbed in the intestine". It should be noted that this needs in some cases to be backed up by method information, e.g. where CHO= CHOT – FIBT and for UK CHO values that include oligosaccharides.

Total carbohydrate

It was noted that "total carbohydrate" [CHOT] did not have a scope note. By analogy with the above, the scope note "Use for total digestible and indigestible carbohydrates, including dietary fibre" was added. This was supplemented by an Additional Information note to the effect that "The EC labelling directive defines fibre as carbohydrate polymers with three or more monomeric units, which are neither digested nor absorbed in the human small intestine." (EC, 2008).

Sugars

The term "mannose" [MANS] was added, specifically for the monosaccharide with the D-configuration. When this was done, it was noted that the INFOODS tagname is the anomalous MAN, which needs to be resolved. The synonyms "saccharose" for "sucrose" [SUCS] and "dextrose" for "glucose" [GLUS] were added. It was suggested that terms for individual added sugars might be added to supplement the overall term "added sugar" [SUGAD], but it was felt that these should be handled as ingredients rather than as components. It should be noted that there are implications for the recipe calculation of SUGAD values if these are not present in the contributing ingredient data (including the ingredient *Sugar*). This issue should be reviewed for version 2.0 of the Component Thesaurus.

During work on the *Polyols* sections below, reference to the monosaccharide D-tagalose was noted (Bär, 2004). It occurs naturally in small amounts in heat-treated dairy products, but it may be more significant as a novel food and sweetener (approved by EU in 2005 but with an energy factor yet to be finalised). A proposed amendment to the definition of 'sugars' seeks to exclude "polyols, isomaltulose and D-tagatose" since isomaltulose and D-tagatose are permitted novel

foods and differ in their physiological properties (EP, 2009). These sugars should be reassessed in future updates for possible inclusion in version 2.0 of the Component Thesaurus.

Resistant starch

Terms were added for the four forms of resistant starch (Sajilata *et al.*, 2006), with codes STARES*n* where *n* = 1 to 4. The general term STARES was given a scope note allowing its use for total resistant starch or if the specific type of resistant starch is unknown. In the INFOODS discussions, it was questioned whether the four forms are required for EuroFIR, but the entries will be retained until a definite decision is taken to remove them.

Polyols

The codes for "polyols, total" and "lactitol" were changed from POLY to POLYL and from LACTTL to LACTL, respectively. In the INFOODS discussions, the alternatives POLYLS and POLYOLS have been suggested, but POLYL will be retained pending any further decisions, possibly for version 2.0. The term "maltitol" [MALTL] has been added, being on the Netherlands' component list. The synonym "glucitol, D-" was added for "sorbitol" [SORTL]. Although the Alditols section of IUPAC recommendations (IUPAC/IUBMB, 1997) states that the trivial name sorbitol is not recommended for D-Glucitol, its use is general in the food area and in food legislation. Therefore "sorbitol" should be retained as the descriptor in the Component Thesaurus.

The basic definition of polyols for EU labelling purposes is "alcohols containing more than two hydroxyl groups" (EP, 2008). A proposed amendment (EP, 2009) would provide the longer definition "*polyols* are defined as carbohydrates which are reduced mono-, di-, oligosaccharides or polysaccharides and which are listed as permitted sweeteners". This amendment is intended to avoid any misunderstanding of the term alcohol and to exclude extraneous compounds, particularly glycerol, as well as to restrict the definition to the context of the legislation to those polyol substances authorised as sweeteners in foods. The thesaurus definitions will need to be reviewed when the legislation is finalised and enacted.

Polysaccharides

The term "hemicellulose" [HEMCEL] was added, being on the Netherlands' component list.

Lipid components

Fats

As the term "triglycerides" is deprecated, it was replaced by "triacylglycerols" in the scope note for "total fat" [FAT].

A new group heading for "Fats" has been created and the terms with codes FAT, FATAN, FATPL and FATUNK moved into it. Following requests for use in Dutch data, the following new terms were added to the group: "saturated fat, total" [FATSAT], "monounsaturated fat, total" [FATMU], "monounsaturated fat, total cis" [FATMUCIS], "polyunsaturated fat, total" [FATPU] and "trans fat, total" [FATTRN]. Codes of the form FATMU have been used for monounsaturated fats, rather than FATMS, since the former is probably clearer (and perhaps benefits from the difference from the FAMS analogy). Scope notes have been added in the form "Use for total *xxx*saturated fat, which includes the contribution of the glycerol moiety as well as the *xxx*saturated fatty acids. Use of the term is deprecated except in old data" for FATMU, FATMUCIS, FATPU, FATSAT and FATTRN. These terms have also been related to the corresponding fatty acid terms. It was noted that these descriptors can be considered a matter of the unit used, analogous to the following discussion.

One type of fat, salatrim, has an energy conversion factors (6 kcal/g, 25 kJ/g) that are lower than the general ones for fat (EP, 2008). Salatrim is an acronym for Short- And Long-chain Acyl TRIglyceride Molecules (FAO, 1997). At present it is not represented in the Component Thesaurus and thus values contributing to an energy calculation cannot be included in food composition data. A further problem with the draft legislation is that although salatrim is fat, fat remains as total lipids and does not exclude salatrim. Potentially, the energy contribution of salatrim is double counted. The situation has some parallels with the issue of added sugars and related novel foods and may need attention during future updates to the thesaurus.

Fat expression as triacylglycerol equivalents

The EuroFIR input to the discussion with INFOODS considered the existing EuroFIR term "fatty acids, total, calculated as triacylglycerol equivalents" [FACIDCTG]. It was noted that the definition incorporates the calculation method used and therefore the term should be deprecated in the EuroFIR thesaurus. However, the more fundamental question is which component is appropriate. Although the descriptor refers to fatty acids, and thus the identifier FACID, the intention of the concept is to provide a more specific measure of "fat" than that of "total lipids" currently equated to "total fat" [FAT]. The value reported is for FAT, with the method "calculated as fatty acid triacylglycerol equivalents".

Comment, PC: No, FAT does not fit here as according to the scope note FAT is for total lipids including non-TAG lipids.

A more appropriate (new) term would be TAG for triacylglycerols, with a scope note indicating that both TAG including glycerol or excluding glycerol in the calculation was used for calculation, which would need to be specified with a corresponding Method Indicator. Two new MI would have to be generated, a "reversed" MI0207 with a formula TAG = total fatty acids X conversion factor, and a new one considering glycerol: TAG = (total fatty acids X conversion factor) + glycerol.

Comment, AM: I agree with Paolo. We have a problem here. I would suggest FATAG. However, here we are taking the completely opposite standpoint than for PROT. .

Further comment, IU: The EuroFIR term FACIDCTG seems to approximate to the US "NLEA fat" and these can be equated to both of the components FAT and FACID. It is a way of expressing either component. In the case of FAT, it is a method-related difference (dependent on the extraction) in the measurement of lipids, which excludes some (e.g. sterols) but includes some contribution of others such as phospholipids. FACIDCTG can also be considered as a way of expressing fatty acids; an analogy can be made with *monosaccharide equivalents* as a unit (or, more correctly, "mode of expression", in the original meaning of the term). However, if some of the fatty acid is present as, for example, phospholipids, the triacylglycerol contribution may be misrepresented (being fatty acid diacylglycerol plus something else) and thus this mode of expression for fatty acids may not be particularly helpful. This area should be reviewed for version 2.0.

Individual fatty acids

In general, extra systematic names have not been added as synonyms at this time for C-1*n* length chains, where the *xxx*adeca name fragment makes these clear. However, they have been added for the longer C-2*n* chains, where the systematic naming may be less familiar. They have also been added where they were included in the version 1.0 descriptor. This creates something of an anomaly with, for example, tridecanoic acid being given as a synonym for F13:0, but not dodecanoic acid for F12:0, although additional synonyms can be added later if required. Extra synonyms have been included for the branched-chain fatty acids.

Codes for individual fatty acids need to be defined with regard to the structural detail that is known for an individual fatty acid. Conventionally, the position of the double bond(s) in unsaturated fatty acids has been represented using the shorthand *n*-notation that counts from

the methyl end of the carbon chain. Strictly (O'Keefe, 2008), *n*-notation assumes that double bonds have a *cis* configuration and, in polyunsaturated fatty acids, are methylene-interrupted, i.e. successive double bonds start three carbon atoms on from the start of the previous double bond (as in the chain fragment $CH{:}CHCH_2CH{:}CH$). In contrast, EuroFIR and INFOODS codes use an explicit indication of configuration with, for example, the codes F18:3CN3, F18:3TTTN3 and F18:3N3 for alpha-linolenic acid, linolenelaidic acid (which is all-*trans*) and 9,12,15-octadecatrienoic acid (used for the total or if the specific geometric isomer is unknown). The codes use "CN" to indicate all-*cis* and F18:3TTTN3 was initially changed to F18:3TN3 to use "TN" correspondingly for all-trans. However, as discussed below for *Polyunsaturated fatty acids*, there are sound reasons for applying differing policies to all-*cis* and all-*trans* isomers and therefore the code F18:3TTTN3 was reinstated for linolenelaidic acid. The definition and codes for totals of *cis* fatty acids and of *trans* fatty acids are discussed in the later section on *Fatty acid totals*.

It is proposed that all specific detail should be ordered (and numbered if necessary) from the carboxylic terminus and that any *n*-notation should terminate the code. The specific definition of *n*-notation as applying to positional isomers that are fully methylene interrupted will be used to avoid specifying the locants for double bonds, where appropriate. Thus F18:3TCCN3 would represent 9-*trans*,12-*cis*,15-*cis*-octadecatrienoic acid, whereas locants are required, for example, for the conjugated isomer 9-*cis*,11-*trans*,15-*cis*-octadecatrienoic acid [F18:3C9T11C15]. All conjugated isomers of known structure should probably be specifically coded in this way; in version 1.0 only the general code F18:2CON is defined for conjugated linoleic acid. The two predominant conjugated isomers have now been added with the codes F18:2C9T11 and F18:2T10C12. A further need for specific coding is mentioned in the later subsection on *Hydroxylated fatty acids*.

Saturated fatty acids

The aggregated term "fatty acid 15:0 + 17:0" [F15+17] is no longer valid and has been marked in the thesaurus as inactive. Terms have been added for short straight-chain fatty acids with the codes F5:0, F7:0 and F9:0 and also for F25:0, hyenic acid. The terms "fatty acid 2:0" and "fatty acid 3:0" have been added as synonyms for "acetic acid" [ACEAC] and "propionic acid" [PROPAC], respectively.

A review of fatty acid data provided in UK analytical reports indicated that sometimes values are given for individual branched-chain isomers and for total C*nn*:0, e.g. "C16:0 iso" and "C16:0 total". This suggests that the figure for the total includes the branched-chain contributions. This should be considered further, for version 2.0, before exact definitions of terms such as F16:0 are incorporated into the scope notes.

Monounsaturated fatty acids

For the monounsaturated fatty acids, pairs of components could be defined for each positional isomer, one with the configuration at the double bond unspecified and the other specified as *cis*, e.g. F18:1N9 and F18:1CN9. It has been suggested that this is necessary, but since version 1.0 exclusively included the cis form, the unspecified form has not yet been added pending a final decision for version 2.0. On the other hand, at present the code F22:1N7 has been retained, although possibly it should be changed to F22:1CN7 to be consistent with the normal policy for existing terms.

For the F10:1 components, the code for caproleic acid (9-decenoic acid) has been kept as F10:1CN1, although this is wrong, because caproleic acid does not have geometric isomers. Similarly, caproleic acid has at present been defined as part of the F10:1CIS sum, although this is not strictly correct.

Terms were added for "fatty acid 16:1 n-9 trans" [F16:1TN9], for "fatty acid 14:1 trans" [F14:1TRS], to correspond with similar terms for other common chain lengths, for "fatty acid 18:1 cis, remainder" [F18:1CR], and for "fatty acids, monounsaturated, total trans" [FAMSTRS]. The descriptor for "fatty acid 18:1 trans n-9 (elaidic acid)" [F18:1TN9] was modified to be consistent

with the other C18:1 isomers. The synonym “vaccenic acid” has been added for *trans*-11-octadecenoic acid [F18:1TN7].

As requested by Norway, the following terms were added: F14:1CN9, F17:1CIS, F20:1CN7, F22:1TRS and F24:1CIS. During this work, the descriptors for F14:1CN5 and F14:1TN5 were modified to be consistent with those for their C16 analogues.

The Dutch data include values identified as “F18:1 (n>12)t” (i.e. *n13 trans* and above) and “F18:1 (n<4)c” (i.e. *n3 cis* and below). If these are to be included in the EuroFIR thesaurus, it is suggested that the letters A and B are used for Above and Below, respectively. Further, it may be better if the code represents an isomer present in the range, so that *X*A reads as “*X* and above” and *X*B as “*X* and below”. This would result in the two codes for the Dutch values being F18:1TN13A and F18:1CN3B, but this policy needs to be discussed and agreed for version 2.0.

Comment, PC1: Principally agree. But are "Above" and "Below" the proper English terms? I would have guessed "Greater" and "Smaller" to be more appropriate.

Comment, IU1: I agree that A and B sound somewhat unscientific (although I think they are valid English). Normally “Greater than” and “Less than” are used together, so perhaps G and L would be best. Perhaps using the two letter forms GT and LT should be avoided, with T already in use for trans and sometimes total.

Comment, PC2: We have LT for less than in the Value Type thesaurus, but also BL for below detection limit. If LT and GT are used, we perhaps need to include them in parentheses (), in accordance to "Condensation products" suggested above. → F18:1(LT)CN3, F18:1(GT)CN3

Comment, IU2: Use of LT and GT perhaps implies use of the non-included limiting statement, e.g. “less than n-4” rather than “n-3 and below”, making the above examples F18:1(LT)CN4 and F18:1(GT)CN12. Susanne has expressed some concern about the length of codes, but unless the EuroFIR identifiers are changed to meaningless codes, clarity requires length.

Polyunsaturated fatty acids

Terms in the polyunsaturated group are more variable than those for monounsaturates and often, intentionally or not, do not fully specify structure. The C16 polyunsaturates only have the general entries F16:2, F16:3 and F16:4. No scope notes indicating the use of more specific terms have been added, but more specific terms should be created when required. In contrast, INFOODS tagnames for C16 polyunsaturates designate double bond position.

Some descriptors have been edited to make them consistent, placing the n-number before the indication of cis-trans configuration. For trienic acids and above, forms such as “cis,cis,cis” have been replaced by “all-cis” or “all-trans”, as appropriate. To standardise on single use of the geometric indicator for all-cis and all-trans forms, the codes F18:2TTN6 and F18:3TTTN3 were initially changed to F18:2TN6 and F18:3TN3, respectively. However, Dutch analytical reports report values for total trans F18:2N6 and F18:3N3, presumably including all isomers with at least one *trans* bond, so possibly a better policy would be to use the shorter forms of F18:2TN6 and F18:3TN3 for the totals of fatty acids having at least one double bond in the trans configuration and the more specific identifiers F18:2TTN6 and F18:3TTTN3 for the all-*trans* forms. This leaves differing policies for all-*cis* and all-*trans* isomers, but as these probably fit better with the data that are normally reported, the code F18:2TTN6 was reinstated.

Many polyunsaturated fatty acids have pairs of codes with the forms F*nn*:*n*N*m* and F*nn*:*n*CN*m*, with the former not specifying the geometric (cis/trans) configuration and the latter indicating the all-cis form. Scope notes have been added to this effect. The descriptor for F18:3N3 was changed from “fatty acid 18:3 cis,cis,cis n-3” to “fatty acid 18:3 n-3”, both to reflect this policy and to differentiate its definition from that for F18:3CN3.

For F18:4N3, “parinaric acid” was deleted as a synonym, as this name relates to conjugated isomers with mixtures of cis and trans double bonds. The synonym “stearidonic acid” was moved from F18:4 to F18:4CN3 as it is used specifically for the all-*cis* compound. Similarly, the

synonym “arachidonic acid” was moved to F20:4CN6 and “timnodonic acid” to F20:5CN3. Currently the codes F20:4CN3 and F21:5CN3 are missing. In the latter case, the synonym HPA was placed with F21:5N3, whereas “heneicosapentaenoic acid” was put with F21:5.

The F22:3 acid is only present as F22:3CN3, with no corresponding more general entries at F22:3 or F22:3N3. F22:4 has general entries of F22:4, F22:4N3 and F22:4N6, but a specific entry only for F22:4CN6. The synonym “clupanodonic acid” was moved from F22:5N3 to F22:5CN3. There seems to be some confusion with the terms “clupanodonic acid” and “clupadonic acid”, with both being used for DPA but the AOCS list[3] giving the former the structure 4c8c12c15c19c-20:5, i.e. with not all double bonds methylene separated. The existing entry for F24:2N6 has been supplemented with terms for F24:2 and F24:2CN6 as the latter is required for the Netherlands data.

The code for “total trans-octadecadienoic acids” was changed from F18:2TN to F18:2TRS for consistency. Various other F18:2 terms need further review and consideration. The intended use of “fatty acid 18:2 iso” [F18:2ISO] was unclear, but USDA documentation suggests that this term was coined for the F18:2 isomers other than linoleic acid [F18:2CN6]. In this case, the meaning is probably the same as “fatty acid 18:2 remainder” [F18:2R]. The code F18:2ISO has been made inactive and “fatty acid 18:2 iso” has been added as a synonym for F18:2R, which now also has the scope note “Use for the total of isomers of F18:2 not separately reported, usually all isomers other than linoleic acid”. The term “isolinoleic acid” is variously used for conjugated isomers and for linolenic acid with its central double bond saturated. If structures of the latter type are required as components, an alternative approach to n-system codes may have to be implemented. Previously, the only term for conjugated isomers was the total “fatty acid 18:2 conjugated” [F18:2CON]. As noted earlier, the two predominant conjugated isomers have now been added with the codes F18:2C9T11 and F18:2T10C12; terms for other specific isomers may also be needed. The preferred term “rumenic acid” and the less preferred “bovinic acid” have been added as synonyms for F18:2C9T11 (Kramer *et al.*, 1998).

As requested by Norway, the following specific terms were added: F16:2CN4, F16:3CN3, F16:4CN3, F20:4CN3, F20:2TN6 and FAPUN3LC. The definition of “long-chain” was modified from “greater than C18” to “C20 and above”.

General terms for trans polyunsaturates have been added as F18:3TRS, F20:3TRS, F20:4TRS, F22:2TRS, F22:5TRS and F22:6TRS, using the 3-letter indicator of the *trans* configuration. However, in accord with the revised policy for specifying *trans* isomers, it is proposed to assign all-trans isomers codes using a “T” for each bond. Thus all-trans eicosadienoic acid (included in the Netherlands’ list) has been assigned the revised code F20:2TT as it specifically represents the all-trans isomer (but N unknown), rather than F20:2TRS, which would represent the more general set of *trans* isomers (at least until the definition of a trans fatty acid is fully agreed).

Hydroxylated fatty acids

Version 1.0 of the thesaurus contained two hydroxylated fatty acids, “fatty acid 18:1 OH n-7 (ricinoleic acid)” [F18:1N9O] and “fatty acid 18:0 dihydroxyoctadecanoic acid” [F18:1TNO]. Ricinoleic acid is 12-hydroxy-9-cis-octadecenoic acid, so the code F18:1N9O designates the remaining double bond as n-9 but leaves the hydroxyl position undefined. The code should be used for this specific isomer, with F18:1N9OX to be defined if it ever necessary to include a code for the component with hydroxyl position unknown. A more specific code following the proposal earlier in this document would be F18:C9O12 for ricinoleic acid, although *in extremis* it might also be necessary to report the (R) configuration of the hydroxy group.

However, the use of an F18:1 code for a saturated compound is considered misleading, as is the T or TN designation (which may be intended to indicate a 9S,10S configuration). The code has been changed to F18:0DO, matching the descriptor. This code has been defined as “Use

[3] http://www.aocs.org/member/division/analytic/fanames.cfm

for total dihydroxyoctadecanoic acid or if isomer unknown", with suffixes to be used in the future for specific enantiomers. Therefore F18:0DO has not been linked to ChEBI:49254, (9S,10S)-9,10-dihydroxyoctadecanoic acid.

Fatty acid aggregations

Although version 1.1 of the Component Thesaurus arranges the terms for components hierarchically, the alphabetical listing of descriptors will remain a major option for viewing the contents. The descriptors for FASAT, FAMS and FAPU are "fatty acids, total *xxx*saturated", which separates these from subtotals such as "cis" and "n-3" but brings them together with totals that include contributions from more than one of the main fatty acid groupings.. The descriptors for all fatty acid aggregations within a main grouping have been revised to forms such as "fatty acids, *xxx*saturated, total *yyy*". It is noted that although there are cis and trans totals for monounsaturated fatty acids, equivalents do not currently exist for polyunsaturates. This perhaps reflects a difficulty in defining cis and trans for polyenes, where the asymmetric definitions of "all-cis" and "not all-cis" may be appropriate to the intended meaning. This point is now resolved in definitions of codes such as F18:2TRS, where such terms include all isomers with at least one *trans* bond and scope notes have been revised to this effect. There is also a lack of clarity in the definition of positional isomerism using n-notation for polyunsaturates.

During the INFOODS discussions, it was noted that the generic codes for unsaturated fatty acids are inconsistent, with FAMS use for MonounSaturated Fatty Acids and FAPU for PolyUnsaturated Fatty Acids. Use of the more logical FAMU was suggested for monounsaturates. As the existing codes have been in use from the introduction of tagnames and are well-established, such a change would need to be in agreement with INFOODS if harmonisation is to be maintained. Some preference for changing from FAMS to FAMU has been expressed, but some fat/FA issues such as this will need to be discussed for version 2.0.

An unresolved difference with INFOODS exists in the preferred policy for specifying codes that qualify the generic fatty acid codes FASAT, FAMS and FAPU. For the simple qualification of the term as cis or trans totals, EuroFIR prefers the three-letter part-codes CIS and TRS, e.g. FAMSCIS and FAPUTRS, as being clearer. On the other hand, INFOODS prefers to use single-letter abbreviations, e.g. FAMSC and FAPUT, presumably for consistency with other codes such as FACN3. Similarly, INFOODS prefers FAPUL to FAPULC for "fatty acids, polyunsaturated, total long-chain" (see below). On the other hand, some EuroFIR compilers have expressed a preference for a wider use of the longer forms CIS and TRS (or TRN). A coherent policy needs to be defined and preferably agreed with INFOODS during the work on version 2.0.

Within the three-letter policy, TRS for *trans* is preferred to TRN in order to avoid any possible confusion with an N used for *n*-notation. The non-preferred form occurred in the code FAMSTRN, which has now been changed to FAMSTRS.

Fatty acid totals

Following requests and suggestions, terms have been added for "fatty acids, total n-3" [FAN3], "fatty acids, total n-6" [FAN6] and "fatty acids, total n-9" [FAN9], the latter included for consistency with the analogous series of FACN3, FACN6 and FACN9. A similar series to that for *cis* isomers has been created for the *trans* analogues FATN3, FATN6 and FATN9. The term "fatty acids, total cis" [FACIS] has been added for completeness.

For "fatty acids, polyunsaturated, total long-chain" [FAPULC], the scope note has been extended to define these as having a chain length greater than C18. This corresponds to the terminology for essential fatty acids, for which short-chain is defined as C18 or shorter. This is different from the general chemical definition for long-chain fatty acids, as exemplified by the ChEBI definition of "Aliphatic monocarboxylic acids with a chain length of C10 or greater". The chain length defined for the ChEBI term "very long-chain fatty acids" corresponds to that for the polyunsaturates total FAPULC. The Norwegian compilers requested a term for "fatty acids, polyunsaturated, total cis". This has been added with the code FAPUCIS, reporting the sum for

the all-cis fatty acids. Analogously, FAPUTRS has been created for the trans total, being the summation of all isomers with at least one trans bond. The term FAPUCIS differs from the term for Polyunsaturates discussed below, because it is not restricted to methylene interrupted isomers.

Based on the preference for using TRS rather than TRN, the code FATRN and FAMSTRN have been changed to FATRS and FAMSTRS, respectively. Terms with the codes FAPUTN3 and FAPUTN6 have been created, limited to the methylene interrupted isomers. The codes FAPUCN3 and FAPUCN6 have also been added, specific to the totals of all-cis, methylene-interrupted isomers for n-3 and n-6, respectively. These can be considered to be related to the more general terms FAPUN3 and FAPUN6 (with the analogous FAPUN9) and these less well-defined terms have been linked to the specific cis and trans totals as Related Terms. The approaches taken should be further reviewed for version 2.0. .

Definitions of fatty acids types

Comment, PC: The scope note of the code FATRN needs to be corrected. *Old*: use for total fatty acids, excluding glycerol. *New*: use for total trans fatty acids, excluding glycerol. A corresponding note for FACIS could be included, i.e. *New*; use for total cis fatty acids, excluding glycerol.

Comment, AM: In European labelling regulations, the definition of monounsaturated and polyunsaturated fat are the sum of cis-monounsaturated fatty acids and cis-polyunsaturated fatty acids, respectively (see the nutrition labelling directive, http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=CELEX:31990L0496:EN:NOT).

The directives Fat and fatty acids definitions are

(f) 'fat' means total lipids, and includes phospholipids;

(g) 'saturates' means fatty acids without double bond;

(h) 'mono-unsaturates' means fatty acids with one cis double bond;

(i) 'polyunsaturates' means fatty acids with cis, cis-methylene interrupted double bonds;

The scope notes should include reference to the nutrition labelling directive.

Further comment, IU: Relating to both these comments, context is significant. The scope note was written within the context of the descriptor, which implies the type of fatty acid. However, the explicit form is better and the scope notes for FATRS and FACIS have been edited, with that for FACIS specifying that only all-cis forms are included. The labelling definitions only apply within the context of the Directive, which might have caused a problem if the differing definition had been applied to the descriptors themselves, e.g. polyunsaturated fatty acids. Fortunately, the modified meanings are associated with modified descriptors, such as *Polyunsaturates*, rather than *Polyunsaturated fatty acids*. The thesaurus should reinforce this difference.

FAPUCISN has been added as the new term “fatty acids, polyunsaturated, total cis methylene-interrupted” for the total conforming to the Labelling Directive, using the strict definition of n- notation to indicate the methylene-interrupted structures. For the general total “fatty acids, total monounsaturated” [FAMS], the sentence “For Mono-unsaturates as defined in the EU Labelling Directive, being fatty acids with one cis double bond, use 'fatty acids, monounsaturated, total cis' [FAMSCIS]” has been added to the scope note. For the general total “fatty acids, total polyunsaturated” [FAMS], the sentence “For Polyunsaturates as defined in the EU Labelling Directive, being fatty acids with cis, cis-methylene interrupted double bonds, use 'fatty acids, polyunsaturated, total cis methylene-interrupted' [FAPUCISN]” has been added to the scope note. The previous Additional Information “Normally limited to isomers with cis, cis-methylene interrupted double bonds but may include trans isomers or alternative positionings, as indicated by the Method Indicator” has been deleted. The synonyms “Mono-unsaturates (EU Labelling Directive definition)” and “Polyunsaturates (EU Labelling Directive definition)” have been added

for FAMSCIS and FAPUCISN, respectively. These changes aim to implement a coherent policy, but need further review for version 2.0.

Further information: The draft legislation (EP, 2008) and the proposed amendments (EP, 2009) incorporate the above definitions, together with that for *trans fat*. The latter is stated as "*trans fat* means fatty acids with at least one non-conjugated (namely interrupted by at least one methylene group) carbon-carbon double bond in the trans configuration". This agrees with the definition in the thesaurus for "fatty acids, polyunsaturated, total trans" [FAPUTRS], but does suggest that possibly the term "trans fat, total" [FATTRN] should not be deprecated. Amendments (EP, 2009) are proposed (with justification in German) for the above definition to become "*mono-unsaturates* means fatty acids with one carbon-carbon double bond in the cis double bond [*sic* - configuration]". More significantly, the proposed definition of polyunsaturates is materially changed to "*polyunsaturates* means fatty acids with at least two isolated carbon-carbon double bonds", removing the requirement for these to be methylene-interrupted (a term that is itself ambiguous). Incidentally, this proposal also suggests using nitrogen conversion factors differing from 6.25 for milk protein and soya protein. The final version of the legislation will need to be carefully checked for any implications for the Component and Method Indicator Thesauri.

Fatty acid others and remainders

In version 1.0, the code fragment indicating a remainder was sometimes "R", but more often "XR". For general remainders, the codes have now been standardised using "XR" and code FAPUCR, which duplicated FAPUCXR, has been deactivated. The more specific remainders, such as F16:1R, have not been changed. Their use and the further documentation required to define the meaning of "remainder" in a particular situation need further consideration for version 2.0.

Other lipid components

Cholesterol

One remaining major difference between EuroFIR component identifiers and INFOODS tagnames is for cholesterol, the former using CHORL and the latter using the basic form CHOL. Some preference for CHOL has been expressed and possibly this change should be considered for version 2.0, after consultation with compilers.

Phosphatidyl choline

The code for Phosphatidyl choline has been changed from CHLMP (a long-standing error) to CHLNP, the INFOODS tagname. The ChEBI link was changed from 16110 to the recent entry 49183. This corresponds to the exact definition in the Thesaurus, as detailed in the scope note and Additional Information text that have been added.

Sphingolipid and Plasmalogen

INFOODS proposes to include the tagnames SPHLIP and PLSGN for Sphingolipid and Plasmalogen, respectively. Sphingolipids contain a long-chain alkenyl moiety based on the amino alcohol sphingosine, which has a 1,3-dihydroxy-2-amino grouping that replaces glycerol. A plasmalogen is an ether lipid where the first position of glycerol has an ether linkage with a straight-chain vinyl residue (i.e. an -O-CH=CH- link). It has been questioned whether these components are required by EuroFIR, although on the other hand it is convenient to maintain compatibility with basic tagnames. SPHLIP and PLSGN have been added, with precise definitions in their scope notes.

Organic acids

The hierarchy for organic acids should be reviewed in a future revision of the thesaurus. At present, the term "organic acids, total" [OA] has the scope note "Use for total of energy-contributing organic acids only". "Energy-contributing organic acids" might be added as a group

heading, although at present this is not possible as an authoritative list of energy-contributing acids has not been located. These were covered by the classic text (Merrill and Watt, 1955, pp 6-7), but neither this nor later documents such as the EU Labelling Directive seem to provide a definition of “organic acid”. In lieu of a more specific definition, fatty acids are organic acids, but it would not be sensible to include these. An appropriate definition will be needed and this should specify, *inter alia*, the shortest chain alkanoic acid that is excluded (presumably butanoic acid).

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 are all covered in the Component Thesaurus except for quinolic acid (pyridine-2,3-dicarboxylic acid) and adipic acid (1,6-hexanedioic acid). These have been added, using the more common descriptor “quinolinic acid” for the former compound and the codes QUINLAC and ADIAC, respectively. The Merrill and Watt report also lists glyoxalic acid (glyoxylic acid, oxoacetic acid, formylformaldehyde), aconitic acid (prop-1-ene-1,2,3-tricarboxylic acid, citridinic acid, etc.; sometimes specifically the *cis* isomer) and malonic acid (propanedioic acid). These three acids do not appear in the present thesauri for EuroFIR or INFOODS, although an INFOODS list from a couple of years ago did propose adding malonic acid with the code MALAC, regardless of the fact that this code is already used in both systems for malic acid. This INFOODS proposal added malonic acid and formic acid “from Slovak table”. Further work on the organic acids will be undertaken for version 1.2 and this will consider if terms for glyoxylic, aconitic, malonic and formic acids should be added to the EuroFIR thesaurus.

Di-keto-cholanic acid

This entry has the anomalous code GULDKAC, which may indicate an unspecified synonym. Otherwise, there is no information on the intended compound(s). Cholanic acid is ChEBI 36237 and cholic acid (ChEBI 16359) is its 3α,7α,12α-trihydroxy derivative. Some reference was found to 3,6-diketocholanic acid, which is structurally similar to the bile acid chenodeoxycholic acid (3α,7α-dihydroxy-5β-cholan-24-oic acid) apart from the position of the second keto/hydroxy group. Hyodeoxycholic acid (ChEBI 52023) is 3α,6α-dihydroxy-5β-cholan-24-oic acid and thus is the tetrahydro analogue of 3,6-diketocholanic acid.

Considering the code (and mostly ignoring the name), it is possible that GULDKAC represents 2,3-diketogulonic acid. This has the formula $CH_2(OH)CH(OH)CH(OH)(CO)_2CO_2H$ and is the inactive product arising when the lactone ring of dehydroascorbic acid is irreversibly opened. Further investigation will form part of the version 1.2 work.

Quinic acid

The code for Quinic acid [(1S,3R,4S,5R)-1,3,4,5-tetrahydroxycyclohexanecarboxylic acid] has been changed from CHIAC to QUINAC, the INFOODS tagname.

Phytic acid

The synonyms "phytate" and "inositol hexakisphosphate, myo-" have been added for “phytic acid” [PHYTAC]. Following the approach taken in the Eurofoods Recommendations thesaurus, PHYTAC is classified as an organic acid, although it is a phosphoric acid derivative. In the review for version 2.0, it needs to be confirmed whether phytic acid should be considered an organic acid. In the meantime, the 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 added.

Phenolic components

Phytoestrogens

The code for Daidzein was changed from DAIDZE to DDZEIN, the INFOODS tagname. Similar changes for Genistein from GENIST to GNSTEIN and for Glycitein from GLYCIT to GLYCTEIN were made. Scope notes containing more systematic names were added for the three components, together with a link to the new ChEBI record (542494) for GLYCTEIN. The code for "Isoflavonoids, total" has been changed from ISOFLAVT to ISOFLVND and the information citing the tagname corrected.

Vitamins and related compounds

Vitamin A components and other carotenoids

The Scope Notes and Additional Information for the terms "all-trans retinol equivalents" and "beta-carotene equivalents" have been extended with further information on the documentation of the calculations.

Carotenoids

The code for "carotenoids, total" was initially changed from CAROTENS to CARTOID, as it was pointed out in feedback that this is the current INFOODS proposal. However, it was later been decided that EuroFIR should retain CAROTENS and thus this change has been reversed. A scope note was also added. However, to match current INFOODS proposals, the codes have been changed for "canthaxanthine" from CANTHAX to CTX, for "lutein" from LUTE to LUTN, for "lycopene" from LYCO to LYCPN[4], for "zeaxanthin" from ZEAXN to ZEA and for "capsanthin" from CAPSA to CAPSCIN. The EuroFIR and INFOODS codes for mixtures of lutein and zeaxanthin are LUTEZEAX and LUTNZEA, respectively. For such mixtures (see earlier section on *Mixtures*), it is proposed that EuroFIR will use the constituent codes combined with an operator, for example "LUTN+ZEA" in this case. Therefore, the existing code, LUTEZEAX, has been made inactive, rather than changing it. The term Astaxanthin has been added as the code ASTAX is agreed by EuroFIR and INFOODS. It was noted that there is inconsistency in carotenoids names ending in "-xanthine", with some having a final "e" and others not. An authoritative list of trivial names (IUPAC/IUB, 1974) uses the form without an "e" and the existing descriptors for CTX and CAPSA have been edited from "-ine" to conform to this policy.

Although terms were added for "beta-carotene, cis" [CARTBCIS] and "beta-carotene, trans" [CARTBTRS] (as these were included in the Netherlands' list and also occur in UK analytical reports), it is now considered that the definition for CARTB should be "all-trans beta-carotene only", in agreement with the INFOODS tagname definition. A scope note stating this has been added for CARTB. Provisionally, the term CARTBCIS has been retained. However, the term CARTBTRS has been replaced by CARTBTOT, to be used for the total of all isomers. Use of this summation should perhaps be deprecated as the cis isomers are generally taken to have half the vitamin A activity of the all-trans form, although possibly having greater anti-oxidant activity. In a future version of the thesaurus, it may be necessary to define an identifier for the factored summation of the *cis* and *trans* isomers, although possibly only total beta-carotene equivalent activity (i.e. CARTBEQ) will be reported.

Further investigation is necessary as more than one *cis* isomer occurs, including the 9-*cis* and 13-*cis* forms. Also 9-*cis* beta-carotene often co-elutes with zeta-carotene in HPLC. Further carotenoids isomers may need to be added to the thesaurus at some stage and various issues relating to carotenoids need further discussion for version 2.0. Also, a recent review (Tang,

[4] In the proposal of changes, the new code was given as LYCN, but the correct INFOODS tagname is LYCPN and the EuroFIR thesaurus has now been changed to match this.

2010) on the bioconversion of dietary provitamin A carotenoids to vitamin A indicates that bioavailability is very dependent on the food matrix, which may involve modifications to relevant Method Indicator terms, if not to the Component Thesaurus.

Retinoids

The INFOODS tagname RETOL is specific to all-*trans* retinol, but the original Eurofoods term for this was "retinol (preformed vitamin A)" and may have been used for values reporting all-*trans* retinol equivalents that include other retinoid contributions. Therefore RETOL is now a depreciated code in the EuroFIR thesaurus, with the two valid entries being "all-trans retinol" [RETOLAT] and "all-trans retinol equivalents" [RETOLTEQ]. It has been suggested that the former one of these should be changed to RETOLT to have the same root as RETOLTEQ, but this has not yet be done (one reason being that the "T" in RETOLT could be mistaken for "total" rather than "trans"). It has also been noted that strict adherence to the EuroFIR policy of excluding units would involve also using the code RETOLAT for "all-trans retinol equivalents", rather than RETOLTEQ or RETOLATE. However, RETOLAT defines a single component, whereas RETOLTEQ is an activity including RETOLAT and other contributors.

Recent discussions have highlighted the IUPAC/IUBMB recommendation (IUPAC/IUBMB, 1983), which defines the terms retinol, retinal and retinoic acid as stereoparents, with these names specifying the all-*trans* stereochemistry. Additional Information has been added for "all-trans retinol" [RETOLAT] noting this for the retinol stereoparent and explaining the use of the explicit form in the descriptor and code. For the aldehyde, the name *retinal* is preferred for chemical usage, but *retinaldehyde* is recommended by IUNS for nutritional usage (to avoid possible confusion with the adjective *retinal*). The synonym "retinal" was added for "retinaldehyde" [RETALD] (INFOODS has duplicate tagnames, RETALD and RETAL). Scope notes have been added for RETALD and RETOLDH specifying the all-trans configuration. For RETALD, the ChEBI link was changed ChEBI from 15035 (retinal) to 17898 (all-*trans*-retinal). Terms requested for the Swiss database have been added for 11-cis-retinal [RETALD11] (using the descriptor "11-cis-retinaldehyde" for consistency), all-trans-retinoic acid [RETINAC] and 13-cis-retinoic acid [RETINAC13]. The synonym "isotretinoin (INN)" was added for RETINAC13 since this is the main ChEBI name, although it is an International Nonproprietary Name mainly relevant to pharmaceutical use.

Terms have not yet been added for individual retinyl esters such as all-trans-retinyl palmitate, all-trans-retinyl oleate, all-trans-retinyl stearate and all-trans-retinyl linoleate. An alternative approach to coding these components has been proposed in the earlier section on *Condensation products*, which would use the identifiers RETOL()F16:0, RETOL()F18:1CN9, RETOL()F18:0 and RETOL()F18:2CN6 for these specific esters. These terms could be added to version 2.0 of the thesaurus to prototype the approach for condensation products, but this will need further discussion.

Reporting values for retinol as the free alcohol alongside values for specific esters implies that two identifiers are required, one for free all-trans retinol and one for total all-trans retinol. It seems likely that the normal use of RETOLAT is for the total and thus a new term is required for free all-trans retinol. Although use of the code RETOLOH is a possibility, there might be possible confusion with RETOLDH. Therefore the term "all-trans retinol, free" [RETOH] is proposed for addition to version 2.0 of the thesaurus, with appropriate scope notes for it and RETOLAT, but this should be discussed before an entry is made, taking into account any relevant method issues.

Comment, PC: Further information on the nomenclature of retinoids is available in IUPAC/IUBMB (1983). There are missing components for calculation of RETOLTEQ (data recorded in the Swiss FCDB), namely all-trans-dehydroretinol (or the existing RETOLDH needs to be modified to RETOLATDH in accordance to the new code RETOLAT), all-trans-retinal (= all-trans-retinaldehyde), 11-cis-retinal, all-trans-retinoic acid, 13-cis-retinoic acid, all-trans-retinyl palmitate, all-trans-retinyl oleate, all-trans-retinyl stearate, all-trans-retinyl linoleate, all-trans-retinyl acetate and "retinols remainder".

And for calculation of CARTBEQ, astaxanthine and “carotinoids remainder” are required.

Comment, AM: Do you get your analysed data as these components or are they actually the substances (nutrients/ingredients) allowed to add to foods in Switzerland? The vitamins and minerals allowed in EU is listed in REGULATION (EC) No 1925/2006, but these are ingredients (food additives) not components. We have another “grey” (overlapping) area here.

Further comment, IU: As I noted earlier, astaxanthin is included as "to be added" now that the identifier is agreed with INFOODS. However, as I understand it, it is not vitamin A active and therefore does not contribute to CARTBEQ, although it is a strong anti-oxidant. The grouping of active and inactive carotenoids has been discussed earlier, but for version 2.0 it must be decided if “carotenoids remainder” refers just to vitamin A active compounds or all carotenoids.

For the retinol esters, I noted the harmonisation problem, in that there are (presumably equivalent) INFOODS tagnames for the acetate and palmitate of VITAACT and VITAPAL, respectively, although the retinol esters should have RETOL-type codes. Also, for version 2.0, it should be considered if all the esters needed or if some are sufficiently handled as ingredients.

Revised discussion for retinoids

Taking the IUPAC/IUBMB recommendations into consideration, one option would be to re-activate the term “retinol” [RETOL] specifically for the all-trans form, thus harmonisiing with INFOODS but duplicating the term “all-trans retinol” [RETOLAT]. In version 1.0, the terms “retinol (preformed vitamin A)” [RETOL] and “all-trans retinol” [RETOLAT] were both valid, but neither had a scope note. In the 1.1 version, RETOL has the scope note “Use only when it is not known if the value reports all-trans retinol [RETOLAT] or all-trans retinol equivalents [RETOLTEQ].”. It must be decided for version 2.0 whether it is necessary to maintain these separate descriptors or to re-define RETOL as the stereoparent “retinol”, with the all-trans configuration, thus harmonising with the INFOODS tagname.

Whichever of these options is taken for retinol, it is preferable to treat the terms “retinaldehyde” and “retinoic acid” as stereoparents. Thus the identifiers RETALD and RETINAC (which is the tagname proposed by INFOODS) are defined in version 1.1 as specifically for the all-*trans* isomers. This represents a differing treatment to retinol as the specific identifier RETOLAT has been retained, but this seems a much better alternative than introducing the new identifiers RETALDAT and RETINACAT.

Published analytical data (Majchrzak *et al.*, 2006) reports compositional values for retinyl esters, together with values for non-esterified retinol (all compounds having the all-*trans* configuration). Component descriptors are required for each ester and for non-esterified retinol. The proposed new terms are “all-*trans*-retinyl palmitate” [RETOLPAL; CHEBI:17616], “all-*trans*-retinyl oleate” [RETOLOLE], “all-*trans*-retinyl stearate” [RETOLSTE], “all-*trans*-retinyl linoleate” [RETOLLIN] and “retinol, non-esterified” [RETOLOH]. These were selected by analogy with VITAACT and VITAPAL (which probably should be deprecated), but are not ideal. For example, there is potential ambiguity between identifiers for the linoleate, alpha-linolinate and gamma-linolinate esters. The Majchrzak paper gives the factored summation for “retinol equivalents” [RE] (or more specifically, RETOLAT as the component identifier):

RE = RETOLOH + RETOLPAL / 1.83 + RETOLOLE / 1.92 + RETOLSTE / 1.93 + RETOLLIN / 1.92

This may be needed as a new Method Indicator descriptor. Both RETOLAT and RETOLOH might be linked to CHEBI:15367 (“all-*trans*-retinoic acid”) and interrelated as **Related Terms** within the Component Thesaurus.. Although “all-*trans*-retinyl acetate” [RETOLACT, CHEBI:32095] was not relevant to this study, it should perhaps be added to the Component Thesaurus at the same time that VITAACT is deprecated.

The terms 11-cis-retinal, 13-cis-retinoic acid and “retinols remainder” have also been proposed. By analogy with RETOL13, the identifiers for the first two might be RETAL11 (CHEBI:16066) and RETINAC9, respectively. ChEBI has 11-*cis*-retinoic acid (CHEBI:46856), but not the 9-*cis* isomer. The term “retinols remainder” should be defined before its identifier is finalised

although, if there is a specific definition, RETOLOT might be used by analogy with FAPUOT ["fatty acids, polyunsaturated, other (= PUFA-linoleic-linolenic)"].

Similarly to carotenoids, there are various issues relating to retinoids that need further discussion for version 2.0. This work would be helped if good reviews on which components are active, on their relative activities, on analytical aspects and the forms used as food additives can be identified.

Vitamin D components

The synonyms "calcidiol" and "calcifediol" have been added for the term "25-hydroxy-cholecalciferol" [CHOCALOH], which is the preferred descriptor for 25-hydroxy vitamin D3. It has been agreed with INFOODS that a corresponding entry for 25-hydroxyergocalciferol is required. The term has been added to the thesaurus, using the analogous code ERGSTROH.

It is noted that the D-provitamin "ergosterol" [ERGSTR] is not included in any calculation method and that the provitamin "7-dehydrocholesterol" is not currently included in the Component Thesaurus.

Vitamin E components

In an approach analogous to that for non vitamin A active carotenoids, all tocopherols and tocotrienols will remain listed in the grouping for *Vitamin E components*, although they may no longer be considered to have vitamin E activity.

The Method Indicator "Vitamin E activity calculated from intrinsic d-alpha-tocopherol and added alpha-tocopherol" [MI0369] refers to two components. However the present scope note of the Component Thesaurus entry for "alpha-tocopherol" [TOCPHA] is "alpha-Tocopherol is defined as RRR-alpha-tocopherol, the only form of alpha-tocopherol that occurs naturally in food, and the 2R-stereoisomeric forms of alpha-tocopherol (RRR-, RSR-, RRS-, and RSS-alpha-tocopherol) that occur in fortified foods and supplements". In effect, it is a simple summation of two components with differing activities, leaving neither of these individually as the definition of a thesaurus term.

Following analogous situations, in particular CARTB being specifically defined as all-*trans* beta-carotene, it is proposed that the descriptor for TOCPHA should be amended to "RRR-alpha-tocopherol" and the scope note revised appropriately. One or more new terms are required for synthetic alpha-tocopherol added to foods. The predominant form is fully synthetic alpha-tocopherol with no control of configuration at C-2, C-4' or C-8', for which the recommended nomenclature is "all-*rac*-alpha-tocopherol" (IUPAC/IUBMB, 1982). This all-racemic product is not necessarily an equimolar mixture of the possible diastereoisomers although usually approximates to it. More specific mixtures may be produced by other approaches, for example alpha-tocopherol with the natural configuration at C-4' and C-8' but both configurations at C-2, such as may be obtained semisynthetically from phytol. The recommended name for this is 2-*ambo*-alpha-tocopherol. At this stage, it is proposed in version 2.0 to modify the descriptor and scope note for TOCPHA and create a new entry for "alpha-tocopherol, all-racemic" [TOCPHARC] (being preferred to TOCPHARAC as this may be interpreted as an organic acid). It is noted that added tocopherol may be in the form as esters such as the acetate or succinate, which should be named with the form tocopheryl rather than tocopherol. Unlike retinol, the name tocopherol is not a stereoparent and carries no implied stereochemistry.

Vitamin K components

"phylloquinone" and "phyllohydroquinone" were added as synonyms of "vitamin K-1" [VITK1] and "dihydro-vitamin K-1" [VITK1D], respectively, and the scope note for the latter was revised. The entry for "menaquinone" [VITK2] was extensively edited, including removal of "(menakinone)" from the descriptor and the addition of a scope note.

Niacin

Better definitions of "preformed niacin" [NIA] and "available niacin" [NIAAVL] are needed, possibly together with extra calculation methods if formulae other than MI0421, MI0423 or MI0424 are used to derive "niacin equivalents" [NIAEQ]. Feedback has raised the question of whether there are three components, i.e. NIA, NIAAVL and NIAEQ, or whether NIAAVL is the same as NIAEQ, i.e. NIA plus tryptophan contribution. Alternatively, NIAAVL may be equal to (NIA – bound NIA). There is a method aspect here, but a problem is that MI0422 [Niacin equivalents calculated from niacin and tryptophan (reduced niacin availability)] applies to NIAEQ rather than differentiating between NIA and NIAAVL.

Possibly NIAAVL can be considered to be the same as NIA, but this will need careful consideration. At present, the scope note for NIA states “Preformed nicotinic acid (usually bound) and nicotinamide” and NIAAVL has no scope note. The Method Indicator thesaurus has calculations for NIAEQ that include NIA with full activity (MI0421), reduced availability (MI0422) and no availability (MI0423). MI0422 is at present tied to a fixed factor of NIA * 0.3. Thus there is no scope to report alternative factors for NIA availability, which might be where NIAAVL could be a useful term. However, there are no MI terms for the calculation of NIAEQ from NIAAVL. This probably needs to be resolved for version 2.0.

Folate components

Terms were added for the specific folates 10-formylfolic acid [FOLFM10], dihydrofolic acid [FOLH2], tetrahydrofolic acid [FOLH4], 5-methyltetrahydrofolic acid [FOLH4ME5], 5-formyltetrahydrofolic acid [FOLH4FM5], 5-methyldihydrofolic acid [FOLH2ME5] and 10-formyldihydrofolic acid [FOLH2FM10]. For substituted hydrofolates, the form of the codes was changed from the original proposals since it is more logical to code the cyclic structure before its substituents, e.g. FOLH4ME5 is used instead of FOLME5H4.

Accurate scope notes are required for the terms “folate, bound [FOLB]”, “folate, free” [FOLFRE] and “folic acid” [FOLACID]. The latter needs to be compared to the INFOODS term “folic acid, synthetic folic acid” [FOLAC]. It has been agreed with INFOODS that EuroFIR will change the code FOLACID to FOLAC, but there should be a final review that they present the same component, which is somewhat ambiguously named in the INFOODS list as “folic acid, synthetic folic acid”. Comments made agreed that this is unsatisfactory. Also, codes need to be designated or assigned for the contributing components in factored calculations of folate, namely “free folic acid”, “bound folic acid”, “intrinsic folic acid” and “added folic acid”. Proposed changes, as described below, have been made, but need to be further reviewed for version 2.0.

Comment, PF: *We should NOT specify conjugated/bound folate but use the terms "Total Folate" to cover the sum of all folate vitamers as monoglutamates, and "Individual Folates as Monoglutamates" to cover folic acid and any other folates being measured separately by HPLC or LC-MSMS etc.*

There is a difference between conjugated (ie polyglutamated forms) and bound (ie mono- or polyglutamates bound to proteins etc). The deconjugation step is very variable and conjugase dependent and what we should be showing total monoglutamate folates in FCDBs as this is the proportion that is nutritionally relevant.

These comments should be reflected in the scope notes of folate terms, with all of these expressed as the monoglutamate. However, further information is required on the definitions for values held in databases.

The terms for folates in the thesaurus hierarchy are:

Vitamins [GRP_VIT]
- Water soluble vitamins [GRP_VITH2O]
  - Folate components [GRP_FOL]
    - 10-formyldihydrofolate [FOLH2FM10]
    - 10-formylfolic acid [FOLFM10]
    - 5-formyltetrahydrofolic acid [FOLH4FM5]
    - 5-methyldihydrofolic acid [FOLH2ME5]
    - 5-methyltetrahydrofolate [FOLH4ME5]
    - dihydrofolic acid [FOLH2]
    - folate, bound [FOLB]
    - folate, free [FOLFRE]
    - folate, total [FOL]
    - folic acid [FOLACID]
    - tetrahydrofolate [FOLH4]

The calculation Method Indicators for folate totals currently defined are:

Calculation methods [MIR002]
- Factored summation [MIR005]
  - Folate calculated from free folic acid and bound folic acid [MI0452]
  - Folate calculated from intrinsic folic acid and added folic acid [MI0453]
- Simple summation [MIR006]
  - Folate calculated by summation of free folic acid and bound folic acid [MI0451]

To handle the contributing values for these calculations, specific definitions for the component terms are required, as noted above. At least one extra term is needed to distinguish between the total intrinsic folate (which is probably better terminology than intrinsic folic acid) and overall total folate, the result of MI0453. The tagname FOLFD is suitable for total intrinsic folate, with FOL used for the overall total. In that case, the INFOODS tagname FOLDFE, dietary folate equivalents, would not be required in the EuroFIR Thesaurus, as it would be represented by FOL + MI0453.

The term “folate, total” [FOL] had the scope note “Use for total folate as determined by microbiological assay”, which did not accord with the definition for "Total Folate" proposed above and also contains method information. The scope note was therefore changed to “Use for total folate expressed as monoglutamate” and an equivalent scope note was added for the individual folate vitamers. However, this reference to the mode of expression was considered inappropriate in definitions in the Component Thesaurus and has been removed. The mode of expression for folate values needs to be confirmed during the version 2.0 work, including whether that total folate values in databases are indeed expressed as monoglutamate.

Initial changes have been made to the Component Thesaurus version 1.1 to support the requirements for handling data used in calculating total folate. The term “folate, food” [FOLFD] has been added for intrinsic folate, compatible with the INFOODS tagname and USDA terminology. The identifier for folic acid has been changed from FOLACID to FOLAC to correspond to the INFOODS tagname and the descriptor changed to “folic acid, synthetic” so that it is specific for added folic acid. The terms for “folate, free” and “folate, bound” have been made inactive and this will also need to be done in the Method Indicator thesaurus for MI0451 and MI0452. MI0453 will need to be checked for compatibility with the expression of values for intrinsic folate expressed as monoglutamate and that the factor used is appropriate for this basis.

Food additives

Policies are needed on components that are included in the Thesaurus as food additives, covering both components that are solely present as additives and those that are also listed in other component groups. That the component is permitted under current EC legislation (EC, 2009) seems a suitable basis. Before this is agreed, an investigation of the implications and

required information should be carried out. For example, it could be decided to include routinely the E-number where appropriate.

Most significantly, policies are needed on which substances that should be considered food components and which should be handled as ingredients. The component listing in the Eurofoods Recommendations gives for the *Additives* heading the scope note "Additives as measured or calculated. Additives as ingredients are handled by food description." However, the list includes salts, which might be calculated from the ingredients, but cannot be analysed (unless the particular salt specified is considered the standard mode of expression for the analytical results). Thus, a newly formulated policy may indicate that the terms for "acesulfam-K" and "sodium-saccharin" should be deprecated in favour of the basic entities acesulfam and saccharin. On the other hand, it may be appropriate to differentiate esters as distinct components, for example having separate entries for each retinol ester. Resolution of these issues will be deferred until version 2.0 is discussed.

Food properties and measures

The terms in this group do not represent food components, but are used to report other numeric values associated with a food. Where these properties are measured, and thus their values have similar numeric and statistical properties as compositional values, their data are conveniently reported within the same data structures. A review should be undertaken of the food properties and measures (e.g. portion sizes and household measures) that are appropriate for this treatment and the corresponding changes made to the Thesaurus version 2.0.

Conversion factors

The EuroFIR Component Thesaurus has terms for "fatty acid conversion factor" [FACF] and "nitrogen conversion factor" [NCF]. However, it was noted in the INFOODS discussions that these are not component identifiers and should be removed from the thesaurus as information on factors is handled in a different way within the EuroFIR data structures. In some circumstances in the past it was found convenient to handle the numerical factors in the same way as compositional values and some compilers may wish to phase out this approach over time. However, NCF and FACF should not be used in the interchange of documented data. Therefore, these terms for conversion factors in the Component Thesaurus have been deactivated, but with appropriate notes on the correct documentation procedures provided in their scope notes. This approach should be reviewed and confirmed before version 2.0 is finalised.

Waste

The EuroFIR identifier for the value of the inedible or discarded proportion of a food is WASTE, whereas the INFOODS tagname is REFUSE. It is unlikely that either can be changed.

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