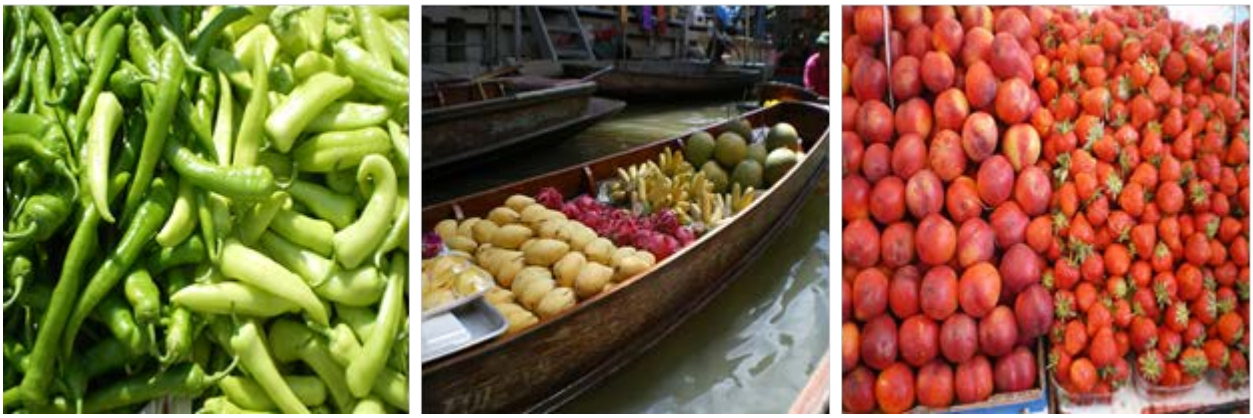
FAO/INFOODS Technical Meeting

Report on the Technical meeting on attributing AOAC methods to INFOODS tagnames

10-11 September 2013 in Granada, Spain



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FOOD AND AGRICULTURE ORGANIZATION OF THE UNITED NATIONS

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I. Acknowledgement

FAO and INFOODS are grateful to the experts for their valuable contribution to the development of the comprehensive list of AOAC method to INFOODS component identifiers, also called tagnames. They devoted an appreciable amount of time and efforts before, during and after the meeting to complete this important task.

Special appreciation is due to Paul Hulshof and Elizabete Wenzel who served as chairs and to Ian Unwin who served as rapporteur. A special thanks goes to FINUT (Fundación Iberoamericana de Nutrición), especially Miguel Fernandez and Angel Gil, for their continued assistance in organizing the meeting in Granada.

The meeting participants express their appreciation for the preparation and execution of the meeting to U. Ruth Charrondiere; to Verena Nowak for the coordination of the working group, which was established for this purpose in April 2013; and Doris Rittenschober for her assistance.

II. Abbreviations

AOAC International	Former names: 'Association of Official Agricultural Chemists', later changed to 'Association of Official Analytical Chemists' and sometimes referred to as 'Association of Official Analytical Community'. However, AOAC International is not an abbreviation
CEN	European Committee for Standardization
DP	Degree of polymerization
FA	Fatty acid
FAO	Food and Agriculture Organization of the United Nations
HPLC	High-performance liquid chromatography
INFOODS	International Network of Food Data Systems
mua	Method unavailable
ORAC	Oxygen Radical Absorbance Capacity

III. Background

When compiling data from different sources, it was noted that it was often difficult to identify the correct INFOODS food component identifiers, also called tagname as the analytical method used was frequently described using solely the AOAC numbers without further indications. As it is assumed that this difficulty is encountered worldwide, FAO/INFOODS decided to attribute AOAC methods to each corresponding tagname. They asked selected experts in food composition and analysis to form a working group to do so. In order to be able to complete this work, FAO subscribed to AOAC International (to be abbreviated as AOAC in this document) and provided free access to all members of INFOODS.

Principles of tagnames

In 1989, INFOODS (International Food Data Systems) published a system to unambiguously identify food components (Klensin et al., 1989[1]). The system ensures a clear, language-independent component identification, which allows users of food composition data to distinguish those component values that are comparable and can be combined from those that are different, even if the component name is similar or the same. The primary objectives for food component tagnames are to identify the component correctly to which a compositional value relates and to determine whether the associated values to components can be compared or combined.

The INFOODS tagnames are like codes or abbreviations according to a specific naming system that allows defining components clearly and unambiguously using only few characters. Tagnames are constructed based on the following requirements and decisions:

1. Each chemical that is analysed should have a unique tagname.
2. The food component tagname scheme should reflect “nutrients”, not just chemistry.
3. Each time an analytical method, expression or calculation is generating significantly different values, a new tagname should be created for the specific component. This ensures that values assigned to the same tagname are directly comparable.
4. Concerning analytical methods, there are three possibilities:
    a. One tagname exists if the different methods provide similar values, e.g. copper.
    b. Several tagnames exist if analytical results are method-dependent. In these cases the method must be a part of the component description, e.g. fibre.
    c. For unknown methods or multiple empirical methods a hyphen after the tagname is used (e.g. FIB-). This is to avoid the assignment to a specific tagname without knowing if it is the correct one.
5. Data of different tagnames cannot be directly compared or combined.
6. Each tagname is a single, unique abbreviation that is intended for use in interchange and databases. Only simple Roman alphabet is allowed in upper case with the addition of a dash “-” or an underscore “_”. Due to the intended use within tags “< >“, the following are not allowed to avoid problems with electronic data interchange:
    a. symbols (: , . % &);
    b. formatting (italics, underlining, subscripts or superscripts);
    c. Greek characters; and
    d. special uses of upper or lower case.
7. The definitions and associated tagnames should reflect the varying importance of method dependency in individual food component definitions.
8. They should allow a language-independent component identification.

[1] John C. Klensin, Diane Feskanich, Victor Lin, A. Stewart Truswell, David A. T. Southgate, Identification of Food Components for INFOODS Data Interchange, Tokyo: United Nations University, 1989

9. The tagname system needs to be robust and extensible to allow new tagnames to be added in the future as both information technology and nutrition science are rapidly developing fields.

IV. Objectives

The objectives of the working group and the technical meeting were the following:

1. Develop a comprehensive list of all possible AOAC methods per tagname;
2. Identify any difficulties in attributing an AOAC method to the corresponding tagname;
3. Identify missing tagnames for components analysed through existing AOAC methods;
4. Identify potential problems in the naming or definition of existing tagnames when attempting to attribute an AOAC method;
5. Identify possible solutions for encountered problems, if possible and time permitting;
6. Publish the list of tagnames and their AOAC method on the INFOODS website, once finalized.

If time permitted, it was intended to discuss component grouping, naming of new tagnames or renaming. However, there was no time during the meeting to discuss these issues in detail. The report will therefore not include these items.

V. Technical discussions

1. General issues

- The priority task of this working group is the attribution of AOAC methods to INFOODS tagnames. Once this task is accomplished, other methods can be added but will for now be added on an ad hoc basis, e.g. CEN (European Committee for Standardization) standards, Journal of AOAC, other internationally recognized methods, or even national methods. The systematic addition of other than AOAC methods would be the task of another working group.

- When no AOAC method can be attributed to a tagname, it should be indicated with “mua” (method unavailable) in order to avoid wrong interpretation of blank cells in the tagname list.

- Tagnames should only be created when necessary. It was decided that this task is to be carried out by the INFOODS Tagname Committee. New tagnames were only suggested for those components for which an AOAC method exists but no tagname. However, they will only be published as official tagname when approved by the INFOODS Tagname Committee. It was agreed that a systematic approach needs to be followed when developing new tagnames.

- A method, which is published as applicable for a feed matrix, should be attributed to tagnames if the food matrix is also used for human consumption (e.g. maize and edible insects can be used for feed or food).

- Methods applicable for nutritional supplements shall be considered as well.

- Methods considered obsolete for a purpose should be still attributed to a tagname and labelled as such (category 2, see below). For reasons of completeness, even obsolete tagnames, e.g. crude fibre (<FIBC>), should be kept in the tagname list while stating in the description that they are obsolete. A comment could be added that the analysis of this component is not useful for human nutrition and analysing these components in foods for human nutritional purposes is considered as a waste of resources. However, even if the tagname is obsolete, the corresponding AOAC method might still be accurate to analyse precisely this obsolete component. E.g. the

AOAC method 920.86 can accurately analyse <FIBC> although <FIBC> is an obsolete tagname/food component for human consumption.

- In order to classify the AOAC methods regarding their applicability, it was agreed to qualify the method attribution using four categories:

1 accurate for purpose
2 obsolete
3 work in progress
4 not enough data to decide yet

Category 1: accurate for purpose
This category includes all methods which are considered accurate for a matrix/purpose, independently whether it is a recently established method or an old one.

Category 2: obsolete
The term "obsolete"[2] in this context refers only to the applicability of the method using the following criteria:

- Inadequate determination of the component
- Hazardous analytical procedure
- Obsolete methods, e.g. according to international standards

Category 3: work in progress
Applies for those methods which have already been established for certain food matrices and which are further expanded to other food groups and matrices, i.e. the same analytical method and instrumentation are used to determine a component in different food matrices which would mean that sample preparation and extraction may differ. The development of new methods is also included in this category. The results are published in the Journal of AOAC but are not classified as official AOAC methods yet.

Category 4: not enough data to decide yet
Due to weak scientific evidence, a clear decision regarding the categorization of a method cannot be taken; not enough information is available on the method. It is not known whether the method is a new method and is going to replace an older method, whether results are comparable with existing method(s) or whether a new tagname needed.

- Since it is not possible to attribute an AOAC method to tagnames which are aggregations or calculations, e.g. <FASAT>, <AAE8>, <PROTCNT>, the general rule was agreed to indicate "see AOAC method of the component(s)" but in cases where this is not appropriate, other options are possible such as "not applicable". For summations, the contributing components must be specified. For activities and other factored calculations, the factors must be specified.

[2] As explained earlier, this is to be differentiated from an obsolete component for nutritional purposes, e.g. crude fibre determination, which should not be used to analyse fibre in foods.

2. Carbohydrates, dietary fibre

Starch

The following tagnames exist for starch: <STARCH> (starch, total), <STARCHM> (starch, total; expressed as monosaccharide equivalents) and <STARCH-> (starch, total, unknown or mixed methods). Originally (Klensin et al., 1989), <STARCH> and <STARCHM> were published as "total starch", even though the comment in the tagname description corresponds to available starch and not to total starch, which should also include resistant starch.

Fifteen AOAC methods are available for total starch, whereas there is none for available starch. Some food composition tables or databases calculate available starch by difference. Therefore, a new tagnames is necessary for available starch, e.g. <STARCHAVL>.

There are five tagnames on resistant starch: <STARES> (starch, resistant), <STARES1> (starch, resistant RS1), <STARES2> (starch, resistant RS2), <STARES3> (starch, resistant RS3) and <STARES4> (starch, resistant RS4). There are no AOAC methods for determining the resistant starch fractions. The AOAC method 2002.02 for resistant starch determination also analyses available starch (used for specific matrix like banana).

Elizabete Wenzel made suggestions to regroup carbohydrates, which was deferred to a subsequent meeting as this was out of the primary scope of the actual meeting. There was no time to discuss component grouping in this meeting.

Agreement

It was agreed to add or modify tagnames as follows:

- <STARCH> starch, total. The sum of all polysaccharides yielding glucose after solubilization with KOH or NaOH and hydrolysis with suitable enzymes; or hydrolysis with acid; includes amylose, amylopectin, glycogen, dextrins and resistant starch. The 15 AOAC methods are to be attached here
- <STARCHM> starch, total; expressed in monosaccharide equivalents. The sum of all polysaccharides yielding glucose after solubilization with KOH or NaOH and hydrolysis with suitable enzymes; or hydrolysis with acid; includes amylose, amylopectin, glycogen, dextrins and resistant starch. Results are expressed in monosaccharide equivalents
- <STARCH-> starch, unknown or mixed methods or expression. It is unknown if total or available starch, and if or not expressed in monosaccharide equivalents.
- <STARCHAVL> starch, available. The sum of all polysaccharides yielding glucose after hydrolysis with suitable enzymes; includes amylose, amylopectin, glycogen, and dextrins

Fibre

A new tagname, representing total fibre including resistant starch and resistant/unavailable oligosaccharides of low molecular weight is considered necessary as there is a new AOAC method available (AOAC 2009.01). A definition for resistant oligosaccharides is needed, which could include carbohydrates with a 3 to 9 DP (= degree of polymerization, number of monomeric units) as composed by resistant maltodextrin, raffinose, stachyose and, fructooligosaccharides (FOS). For this method, the tagname was proposed as <FIBTGLC> which still needs some discussion. This method does not seem to be finalized, therefore the Prosky and similar methods <FIBTG> remain recommended for food composition purposes.

Regarding the two fibre fractions, soluble and insoluble fibre, it is not recommended to separate them. However, since methods for each fraction exist, they should be attributed to the

corresponding tagnames. As AOAC method 2011.25 captures different components, new tagnames seem necessary for soluble and insoluble fibre fractions deriving from this method.

The component <FIBC> is obsolete for human nutrition. However, the respective AOAC is appropriate for the purpose of measuring crude fibre and will therefore be kept for historical reasons and as unfortunately, it is still analysed.

The AOAC methods 997.08 and 999.03 can be attributed to <FRUTN>, but not to <GF2>[3], <GF3>[4], <GF4>[5] and <INULIN>. The methods do not separate fructans by different units of monosaccharides. For <GF2>, <GF3>, <GF4> and <INULIN> there are no AOAC analytical methods, but other methods could be used[6] [7].

Agreement

- Three new tagnames are needed for dietary fibre:
    - representing fibre ≥3DP corresponding to the AOAC method 2009.01 and 2011.25 (final tagname to be determined);
    - soluble fibre corresponding to AOAC method 2011.25 (if proven to be significantly different from existing tagname <FIBSOL> fibre, water-soluble);
    - insoluble fibre corresponding to AOAC method 2011.25 (if proven to be significantly different from existing tagname <FIBINS> fibre, water-insoluble); and
- A definition for resistant oligosaccharides is needed.

Sugars

AOAC methods for sugar are valid and accurate for the purpose.

3. Protein and amino acids

AOAC Method 994.12 describes the determination of *Amino Acids in Feeds*; the same process is applicable to foods. As the acid hydrolysis of proteins destroys cystine <CYS> and partially degrades methionine <MET>, this is preceded by performic acid oxidation, which oxidises these amino acids to cysteic acid and methionine sulphone, respectively. Asparagine <ASN> and glutamine <GLN> are converted by acid hydrolysis to aspartic acid <ASP> and glutamic acid <GLU>, respectively. Thus the values for ASP and GLU often include the contributions from ASN and GLN. Tyrosine <TYR> is destroyed by the oxidation and has no AOAC method. Tryptophan <TRP> is destroyed by hydrolysis, but can be determined by AOAC Method 988.15, *Tryptophan in Foods and Food and Feed Ingredients*.

The question arouse on whether all tagnames representing a combination of several individual amino acids are needed.

[3] 1-kestose (1-kestotriose); one type of fructo-oligosaccharides (FOS): 2 units of fructosyl-fructose link with one unit of glucose

[4] nystose (1,1-kestotetraose); one type of fructo-oligosaccharides (FOS): 3 units of fructosyl-fructose link with one unit of glucose

[5] 1F-β-fructofuranosylnystose (1,1,1-kestopentaose); one type of fructo-oligosaccharides (FOS): 4 units of fructosyl-fructose link with one unit of glucose

[6] Agopian RGD, Purgatto E, Cordenunsi BR, Lajolo FM. Synthesis of fructooligosaccharides in banana prata and its relation to invertase activity and sucrose accumulation. Journal of Agricultural and Food Chemistry. 2009; 57: 10765-71.

[7] Lajolo FM, Agopian RGD, Soares CA, Purgatto E, Cordenunsi BR. Identification of fructooligosaccharides in different banana cultivars. Journal of Agricultural and Food Chemistry. 2008; 56: 3305-10.

Tagnames for protein quality exist, but these were defined a long time ago. It was questioned whether they were still useful for food composition purposes. If they are to be retained, newer protein quality tagnames need to be added.

Agreement

- A new tagname needs to be included in the list: PDCAAS (Protein Digestibility Corrected Amino Acid Score).
- Tagnames representing a combination of several individual amino acids are "not important" but should be kept as tagnames due to historical reasons.

4. Fat

The definition of "total fat" was discussed. The term fat is used in a very loose way and, depending on the definition and method of analysis, different entities might be included. Especially the sample preparation plays a crucial role, if e.g. prior to extraction acid hydrolysis was carried out or not. So far, all methods go under the same tagname <FAT> (fat, total) except for the Soxhlet method, for which a separate tagname exists <FATCE> (fat, total; derived by analysis using continuous extraction). It was discussed whether method-depend tagnames are needed for fat to capture the methodological differences. It is assumed that Soxhlet and other methods provide similar results if used appropriately which includes acid hydrolysis and the matrix considerations. However, it is difficult to decide which matrices provide similar results. This would be a good proposal to AOAC to investigate this issue further.

The assignment of methods to the two tagnames <FAT> and <FATCE> was not finished yet.

Agreement

- Work on total fat needs to be completed.
- The discussion of the necessity of the method depended tagname <FATCE> was postponed.

5. Fatty acids

There are 24 AOAC methods available for fatty acids (FA). Currently, about 290 tagnames for fatty acids exist. The difficult task is, to find out which FAs and isomers are covered by which of the methods as this also depends on changes in the application of the same method (e.g. longer columns will be able to differentiate more clearly between FAs and isomers).

It was discussed whether to assign obsolete methods for (individual) fatty acid determination, e.g. packed columns, titrimetric and spectroscopic methods (considered as old and not trustworthy).

There is a need of prioritization, firstly, on the level of component identification and secondly, on the level of the importance for human consumption.

Agreement

- Obsolete methods should be assigned to tagnames for completeness and labelled accordingly (category 2).
- Efforts should be focused on FAs relevant for human nutrition rather than on rare and "fancy" FA. Analytical methods for not prioritized FAs shall be labelled with "still to be determined".

6. Ash, alcohol

No difficulties or discussion points were encountered regarding the assignment of methods to <ASH> and <ALC>.

7. Minerals

AOAC methods were found for 36 minerals including radioactive isotopes. No methods were found for 8 elemental tagnames and 35 species minerals.

It was discussed whether the radioactive components strontium-90 (<SR90>), cesium-137(<CS137>) and plutonium-239 (<PU239>) should be kept in the list of tagnames. It was noted that different isotope components are not yet included in nutrient databases. Furthermore, it was discussed if other toxic components such as methyl mercury (<HGME>) should be excluded from the list as they are of importance for food safety, but not for nutrition. A possible indicator for exclusion of a component could be the existence of maximum tolerated dose (MTD) of chemicals.

Two types of element speciation that are represented in existing or proposed tagnames are inorganic/organic speciation and oxidation number speciation, for example for arsenic. There are existing tagnames for total inorganic and total organic arsenic, namely <ASIO> and <ASO>, respectively. The tagnames <AS3> and <AS5> have been proposed for the elemental species of arsenic oxidation states As(III) and As(V). These species occur as arsenite and arsenate forms As(III) and As(V), respectively, which are both oxygen-containing anions.

Agreement

- It was decided to consider excluding radioactive isotopes from the list of tagnames.
- Toxic components mainly considered in food safety will still be kept in the list of tagnames. The decision of inclusion/exclusion of toxic components to be included was postponed.
- The concept of speciation should be retained but is not seen as a priority for the attribution of methods.

8. Water-soluble vitamins

Thiamin

Thiamin is generally analysed by fluorometric method and HPLC (High-performance liquid chromatography). The methods use thiamin hydrochloride as the calibration standard but it can be estimated as thiamin from the beginning or at the final step. Thus, the results can be expressed as thiamin hydrochloride or as thiamin. AOAC methods expressed the results as thiamin-hydrochloride, whereas the CEN standards include the additional step to transform data from the thiamin-hydrochloride to thiamin.

The question was raised as to whether it would be more correct to attribute the AOAC methods to <THIAHCL> and add a comment for <THIA> (thiamin), e.g. “see <THIAHCL> (thiamin hydrochloride), expressed or calculated as <THIA>“.

<THIANO> is used as a food fortificant. It needs to be researched whether it can be analysed as such.

Agreement

- Methods 957.17 (Foods), 953.17 (Grain products, enriched flour, farina, corn meal, macaroni, and noodle products, or where bound thiamin or thiamin pyrophosphate is not significant),

986.27 (Milk based infant formula), 942.23 (Human and pet food) and 938.12 (Vitamin preparations) will be attributed to the tagname <THIAHCL>. The following descriptions will be used:
    - <THIAHCL> thiamin hydrochloride – description: vitamin B1 analysed and expressed as thiamin hydrochloride;
    - <THIA> thiamin – description: vitamin B1 analysed and expressed as thiamin;
- It needs to be checked, whether <THIANO> can be analysed in foods as such.

Folate

The assignment of AOAC methods for total folate needs to consider both the extraction (i.e. single/di-/tri-enzymatic) and the methods of measurement and the method of measurement. Different tagnames exists for total folate and its vitamers. Total folate determined by microbiological assay <FOL> is differentiated from those using HPLC and similar methods <FOLSUM>.

Total folate analysed using HPLC and the like implies the determination of the individual folate vitamers which are subsequently summed up and expressed as the sum of folate vitamers.

A new official AOAC method, which is an optical biosensor assay (2011.05), measures total folate but it was not further investigated if it gives comparable results with other methods. It needs to be further studied what is actually measured, if results are comparable, and to which method.

A new tagname was suggested for 10-methyl folic acid, <FOLME10>, where its format is in alignment with already existing tagname. The AOAC method 2011.06 will be assigned to this new tagname.

Both methods (microbiological assay as well as HPLC) can be used to determine food folate, but <FOLFD> refers to the microbiological method (as used in the USDA national nutrient database).

For the tagname <FOLSUM> (folate, sum of vitamers, determined by HPLC) it still needs to be decided if a method number can be assigned or if it will be stated “see AOAC method for individual component(s)”, which are in this case the individual vitamers analysed with HPLC (AOAC 2011.06).

<FOLH2> (dihydrofolic acid): the short description in the tagname list needs to be checked, whether it refers to folate or folic acid.

The use of “folic acid” should be restricted to synthetic folate used in fortification. However, it is acceptable to use the chemical name “folic acid” in component naming.

<u>Agreement</u>

- The tagname <FOLME10> was created. The AOAC number 2011.06 corresponds to this tagname.
- A new method, optical biosensor assay (AOAC 2011.05), is available. No decisions can be taken yet whether results are comparable with other methods or if a new tagname is necessary. Ttherefore, so far no tagname will be created. “Appropriate tagname to be attributed” will be added to this method.
- So far, tagnames do not differentiate the extraction method (single-, double-, trienzymatic). At present, there is no definite conclusion whether the folate values resulting from different enzymatic treatments are significantly different. More research with specific objective on this issue must be undertaken.
- <FOLSUM>: for method 2011.06 the category “in progress” will be assigned;
- <FOLDFE>: add comment “see AOAC methods for the component(s)”;
- <FOLFD>: add “microbiological method” to the tagname description.

Vitamin B_6

Several tagnames for Vitamin B_6 and components are available:
<PYRXL> (pyridoxal), <PYRXM> (pyridoxamine), <PYRXN> (pyridoxine), <PYRXNHCL> (pyridoxine HCl), <VITB6-> (vitamin B_6, total, unknown), <VITB6A> (vit B_6, total, by analysis) and VITB6C (vitamin B_6, total; calc.).

Analogous to thiamin, vitamin B_6 is normally analysed using pyridoxine hydrochloride as the standard. As a result, the vitamin B_6 content is expressed as pyridoxine hydrochloride or pyridoxine. The AOAC method 2004.07 expressed the total vitamin B_6 as pyridoxine hydrochloride and not as pyridoxine. The CEN Standard goes one step further and describes the calculation to obtain pyridoxine. It was discussed whether values generated in this way should be assigned to <PYRXNHCL> (pyridoxine hydrochloride) or whether this tagname should be renamed to vitamin B6 expressed as pyridoxine hydrochloride.

The tagname <VITB6A> (vitamin B-6, total; determined by analysis) or its description should be reformulated. It would create confusion because all individual vitamers or the total vitamin B_6 content in a food (as determined by microbiological assay AOAC 985.32) needs to be analysed. The CEN Standard description of the method is more complete than the AOAC description as it includes the final conversion to vitamin B_6 values.

It was further discussed whether it is sufficient to refer to "see AOAC method of individual component(s)" with the tagname <VITB6C> (vitamin B-6, total; calculated by summation) or if a further indication is needed for the user to trace back to the actual hydrochloride form.

Agreement
The following proposition needs to be finalized and/or confirmed by the tagname committee:

- The description of the tagname <VITB6A> to be changed to "Vitamin B_6, total, determined and expressed as pyridoxine".
- A tagname is needed to express vitamin B6, total, expressed as pyridoxine-hydrochloride, e.g. <VITB6AHCL>.

9. Fat-soluble vitamins

Several CEN methods exist for fat-soluble vitamins but only few AOAC methods. When CEN and national standards were already attributed to tagnames, this information was kept.

The only AOAC method related to vitamin E is ''AOAC 992.03, *Vitamin E Activity (All-rac-alpha-Tocopherol) in Milk-Based Infant Formula''*; there are no AOAC methods for tocotrienols. The British Standard ''EN 12822:2000, *Foodstuffs. Determination of vitamin E by high performance liquid chromatography. Measurement of α-, β-, γ- and δ-tocopherols''* is a method that determines the tocopherol isomers. All-racemic alpha-tocopherol has a different vitamin activity than other naturally occurring alpha-tocopherol and it was suggested to create a new tagname for it. No AOAC methods exist for tocotrienols.

There are several recent AOAC chromatographic methods for determining the vitamin D vitamers cholecalciferol and ergocalciferol, although the British Standard ''EN 12821:2009, *Foodstuffs. Determination of vitamin D by high performance liquid chromatography. Measurement of cholecalciferol (D3) or ergocalciferol (D2)''* is more developed. A standard method for determining the more active 25-hydroxy derivatives is not yet available.

For vitamin K, AOAC 999.15 (*Vitamin K in Milk and Infant Formulas*) provides for the determination of vitamin K_1 and further modifications are under development. The British Standard ''EN 14148:2003, *Foodstuffs. Determination of vitamin K1 by HPLC''* is also available.

For carotenoids, AOAC method 2005.07 ''β-*Carotene in Supplements and Raw Materials''*, specifically determines all-*trans*- and total β-carotene. The method description does cite retention times for other carotene isomers, but the remaining carotenoids might be changed to "no AOAC". The *cis* and *trans* isomers of β-carotene have different activities, although the *cis* form may partly be formed by isomerisation from the *trans* configuration. It was noted, that the tagname description of cryptoxanthin <CRYPX> (cryptoxanthin) should be more refined, specifying that this tagname refers to total cryptoxanthin. The tagname for β-cryptoxanthin, <CRYPXB>, should be defined to include only the all-*trans* form.

Methods for the retinoids have not yet been attributed.

Agreement

- CEN methods already attributed to tagnames will be kept.
- <CRYPX>: tagname description should be more refined; "cryptoxanthin, total";
- <CRYPXB>: tagname description should be more refined; "all-trans beta-cryptoxanthin".

10. Polyols and organic acids

The main discussion regarding this component group was about missing definitions for organic acids and polyols. The EU directives on nutrition labelling for foodstuffs (90/496/EEC), last amended by EC Regulation 1137/2008, require the calculation of energy to include the contribution of organic acids (3 kcal/g) and of polyols (2.4 kcal/g), other than erythritol (0 kcal/g). A polyol is defined as an alcohol containing more than two hydroxyl groups, but there is no definition of an organic acid.

The main organic acids occurring in foods are citric, malic, lactic and acetic acids, with formic, fumaric, maleic, malonic, oxalic, quinic, shikimic, succinic and tartaric acids also occurring, as do 2- and 4-hydroxybenzoic acid (the former being salicylic acid). Butyric acid (F4D0) is considered the shortest chain fatty acid, rather than an organic acid. In addition, benzoic, isoascorbic, propionic and sorbic acids are commonly used as food additives. Many of the AOAC methods for organic acids measure the amounts in various food matrices of those used as additives, including naturally occurring ones such as citric acid. In many cases, both an acid and several of its salts are permitted additives and it is unclear whether only the acid or the total anion should be reported (particularly when the function of the additive is acidity regulation).

Polyols are also known as sugar alcohols, although the >2 hydroxyl groups definition is probably broader than that. Almost always they are present as food additives, for example as sweeteners or humectants, and the *Codex Alimentarius* International Numbering System (INS) for additives could form the basis for deciding the individual compounds (sorbitol, xylitol, mannitol, isomalt, maltitol, lactitol and hydrogenated glucose syrup) to be included in the total polyols <POLYL> value. Polyols such as maltitol and lactitol are based on two sugar units and isomalt is an equimolar mixture of two such compounds (glucopyranoside-sorbitol and pyranosoyl-mannitol), for which tagnames are needed.

AOAC methods exist for glycerol, inositol, sorbitol and xylitol.

Colorimetric and gravimetric methods might be classified as obsolete.

Elizabete Wenzel suggested taking the definition for polyols as proposed by Livesey (2003)[8].

Agreement

- Two new tagnames will be added for glucopyranoside-sorbitol and pyranosoyl-mannitol.
- The discussions on the definition of organic acids and how to separate natural occurring components and additives is postponed. It should be discussed in the tagname committee.

11. Bioactive compounds

For ORAC (Oxygen Radical Absorbance Capacity) some recent methods are provided by AOAC (2012.03, 2012.04, 2012.23) but initially ORAC was not listed for this assignment as there is an ongoing discussion on whether ORAC values in foods are valid. However, recent AOAC methods are available and, therefore, ORAC will be added to the list.

Very recent methods relating to the antioxidant activity of bioactives include AOAC 2012.04 (*Antioxidant Activity in Foods and Beverages*) based on the reaction with 2,2'-diphenyl-1-picrylhydrazyl <DPPH>, AOAC 2012.03 (*Antioxidant Capacity of Commercial Beverages*) for ORAC and AOAC 2012.23 (*Total Antioxidant Activity*) for ORAC using fluorescein as the fluorescence probe.

The analysis of total phenolics covers all reducing compounds including polyphenols and further bioactive substances which lead to the finding that a new tagname is needed. The proposed tagname for total polyphenolics <POLYPHENT> may not be ideal for what is described in AOAC method 965.31 as the total might include similar bioactives that are not polyphenols. Also, the total to be expressed may not be a straight summation and may need to be named as an activity.

The definition of total tannins <TAN> needs to be more specific.

It was noted that many of the methods for bioactives are very old.

Agreement

- Because the proposed tagname <POLYPHENT> did not seem acceptable, a new tagname for representing total reducing components (AOAC 965.31) will be created. Isabel Castanheira will assist Deborah Bastos creating a tagname with an appropriate description.
- No agreement on ORAC was achieved.

[8] Livesey G (2003) Health potential of polyols as sugar replacers, with emphasis on low glycemic properties. *Nutr Res Rev* 16(2): 163-91.

VI. Future work (until mid-2014)

Follow-up: Attribution AOAC methods to INFOODS tagnames

Update of Excel working document by Verena Nowak

- Update of Excel worksheet with incorporation of major decisions and findings that were agreed on during the technical meeting.
- All changes are to be highlighted in yellow (yellow filling of the cell).

All members of working groups

- Finish/update own component group based on the updated Excel worksheet sent out by Verena Nowak
- Attribution of the categories regarding the applicability (1-4) to the methods. In addition, the reason should be stated when category 2 "obsolete" is chosen.

All members of working groups

- Peer-review/validation: It was agreed that the initial peer-review is carried out by members of the working groups and, if needed, additional external experts and reviewers will be identified and consulted. The review should comprise checks on the attribution of the method to a tagname by the first person/working group and whether a method is missing or not. If any discrepancy arises regarding the attribution of methods to a tagname, the reason of the suggested change should be explained. In addition, the allocation of the 4 categories regarding the method applicability should be checked.
- All members of the working group were asked to highlight all changes in yellow (yellow filling of the cell).

The peer review task was assigned as follows:

Isabel Castanheira	Water-soluble vitamins, carotenoids
Paul Hulshof	Fat-soluble vitamins excl. carotenoids
Deborah Bastos	Fatty acids
Kunchit Judprasong Prapasri Puwastien	Ash, moisture, protein, total fat, dietary fibre, carbohydrates
T. Longvah	Minerals
Elizabete Wenzel	Phytochemicals
Ian Unwin	Alcohol
Isaac Akinyele	Amino acids
Verena Nowak, Ruth Charrondiere, Doris Rittenschober	Polyols/organic acids

VII. Further Issues/Recommendations

- A new version of the AOAC book is published every four years, which subsequently results in the need for a regular revalidation of the already assigned quality categories. Especially the methods under category 3 “in process” might have to be shifted to the group of validated methods.

- Due to the need to use the Journal of AOAC INTERNATIONAL in the work, it is recommended that FAO subscribes to it and makes it available to INFOODS and members of the working group in order to fulfil their tasks.

- It was noted that there are copyright problems for CEN and national standards as usually these must be purchased and the reproduction of their text may be restricted.

Annex 1

List of Participants

Name of participant	Component group, for which AOAC methods were attributed	Affiliation
Experts		
Isaac Akinyele	Minerals	Department of Human Nutrition University of Ibadan Ibadan, Nigeria
Deborah Markowicz Bastos	Phytochemicals	Nutrition Department School of Public Health University of Sao Paolo Sao Paolo, Brazil
Isabel Castanheira	Fat-soluble vitamins	Food and Nutrition Department National Institute of Health Doutor Ricardo Jorge Lisbon, Portugal
Paul Hulshof	Fat-soluble vitamins, carotenoids, fatty acids	Division of Human Nutrition Wageningen University Wageningen, Netherlands
Kunchit Judprasong	Minerals	Institute of Nutrition Mahidol University Bangkok, Thailand
T. Longvah	Protein including total nitrogen and amino acids, fat, alcohol, ash, phytochemicals	Food Chemistry Division National Institute of Nutrition Hyderabad, India
Prapasri Puwastien	Water-soluble vitamins	Institute of Nutrition Mahidol University Bangkok, Thailand
Louwrens Smith *	Water-soluble vitamins	Agricultural Research Council Irene Pretoria, South Africa
Ian Unwin	Polyols, organic acids	Cambridge, UK
Elizabete Wenzel	Carbohydrates, dietary fibre, energy	Department of Food and Experimental Nutrition Faculty of Pharmaceutical Chemistry University of Sao Paolo Sao Paolo, Brazil
Secretariat		
Ruth Charrondiere		Nutrition Division FAO Rome, Italy
Verena Nowak		Nutrition Division FAO Rome, Italy
Doris Rittenschober		Nutrition Division FAO Rome, Italy

* Absent from the meeting but contributed to the working group

Annex 2

Draft Agenda for Technical meeting on attributing AOAC methods for INFOODS tagnames
10-11 September 2013 in Granada, Spain

10 September		
9.00-9.15	Welcome and objectives Election of chair and rapporteur Group photo	Ruth Charrondiere
9.15-9.30	Introduction	Verena Nowak
9.30-10.00	General questions	Verena Nowak
10.00-10.30	Ash/alcohol	T. Longvah
10.30-11.00	Protein and amino acids	T. Longvah
11.00-11.30	Coffee break	
11.30-12.15	Fat	T. Longvah
12.15-13.00	Fatty acids	Paul Hulshof/ T. Longvah
13.00-14.30	Lunch	
14.30-15.30	Carbohydrates	Elizabete Wenzel
15.30-16.00	Dietary fibre	Elizabete Wenzel
16.00-16.30	Coffee break	
16.30-17.30	Minerals	Kunchit Judprasong/ Isaac Akinyele
17.30-18.00	Polyols, organic acids	Ian Unwin
> 20.00	Social dinner	
11 September		
9.00-11.00	Water-soluble vitamins	Prapasri Puwastien
11.00-11.30	Coffee break	
11.30-13.00	Fat-soluble vitamins	Paul Hulshof/Isabel Castanheira
13.00-14.30	Lunch	
14.30-16.00	Phytochemicals	Deborah Bastos/T. Longvah
16.00-16.30	Coffee break	
16.30-17.30	Future steps and recommendations	Verena Nowak/ Doris Rittenschober/ Ruth Charrondiere
17.30-18.00	Closing	Ruth Charrondiere
> 20.00	Social dinner	

Report on the Technical meeting on attributing AOAC methods to INFOODS tagnames

10-11 September 2013 in Granada, Spain

Job Number I3784E/1/05.14