Report of the INFOODS/EuroFIR AISBL Workshop on Component Identifiers

held on 17 September 2011 in Norwich as a satellite to the 9th International food Data Conference (IFDC)

Chairs: Ruth Charrondière (RC), Ian Unwin (IU)

Participants:

	Name of participant	Institution
1.	Ruth Charrondière (RC)	FAO/INFOODS
2.	Barbara Stadlmayr (BS)	FAO/INFOODS
3.	Paul Finglas (PF)	EuroFIR AISBL, IFR
4.	Paolo Colombani (PC)	EuroFIR AISBL, ETH Zurich
5.	Simone Bell (SB) – Acting rapporteur	EuroFIR AISBL
6.	Ian Unwin (IU)	EuroFIR AISBL, IDUFIC, UK
7.	Adriana Blanco (AB)	LATINFOODS, Costa RICAFOODS
8.	Elisabete Wenzel Menezes	University of Sao Paulo, BRASILFOODS
9.	T. Longvah	SAARCFOODS
10.	Hettie Schönfeldt (HS)	AFROFOODS advisor
11.	Christiant Kouebou	CAFOODS
12.	Nahomi Imaeda	Nagoya-Wromeins University, Japan
13.	Gerald van Noort	SAFOODS
14.	Prapasri Puwastien (PP)	ASEANFOODS
15.	Susanne Westenbrink	RIVM
16.	Luisa Oliveira (LO)	INSA
17.	Mustafa Yaman	Tübitak MRC
18.	Joanne Holden	NORAMFOODS (USDA)
19.	Jayne Ireland (JI)	Danish Food Information
20.	Hoi Shan KWAN	The Chinese University of Hong Kong
21.	Maria de Lourdes Samaniego	San Pablo – CEU University
22.	Mariana Santos	INSA
23.	Maria da Graça Dias	INSA
24.	Pamela Pehrsson	USDA
25.	Petro Wolmarans	MRC South Africa
26.	Joelaine Chetty	MRC South Africa
27.	Klaus Englyst	Englyst Carbohydrates, UK
28.	Takeshi Yasui	Naro West. Reg. Agric. Res. Cent.
29.	Jenny Plumb (JP)	IFR

Agenda (prepared by Ian Unwin)

09.00 – 09.10 **Introduction**

09.10 – 10.30 **General issues**
- Scope and requirements
- Coverage policies
- Code definition principles
- Component grouping
- Scope notes and other documentation
- Decision making process

10.30 – 10.45 **Carbohydrates**
- Oligo- and polysaccharide definitions

10.45 – 11.05 Coffee/tea

11.05 – 11.25 **Lipid components**
- Individual fatty acids
- Fatty acid totals

11.25 – 11.40 **Vitamins**

11.40 – 12.00 **Bioactives**
- Coverage by INFOODS and EuroFIR
- Code policies

12.00 – 12.20 **Speciation** (oxidation state, ionic species, radicals)
- Coverage
- Code policies

12.20 – 13.00 **Future plans and activities**
- INFOODS tagnames
- EuroFIR component identifiers
- Continuing tagname-identifier harmonisation

13.00 **Close of meeting**

Executive Summary

A background document (see annex 1) was prepared by Ruth Charrondiere and circulated to the foreseen participants of the meeting on 13 September 2011. During the IFDC, it was decided to open the meeting to observers interested in the topic. Ian Unwin prepared a PowerPoint Presentation based on the background document with some additional topics to be discussed (available at http://www.fao.org/infoods/tagnames_en.stm)

This meeting is a continuation of the common work on food components identifiers as decided at the previous meeting, which took place in 2009 in Bangkok as a satellite to the 8th IFDC.

Collaboration on harmonization process on component identifiers between INFOODS and EuroFIR (AISBL)

At the last Component Identifier Meeting in Bangkok in 2009, EuroFIR and INFOODS decided to collaborate on component identifiers and to share their changes and additions prior to publication. INFOODS did share with EuroFir.

Agreement: In the future, both organizations will share their new versions of component identifiers at least one month before the foreseen publication to allow necessary discussion within and between organizations.

General naming of component identifiers

Agreements: INFOODS and EuroFIR will try to harmonize while accepting that few issues remain different:

1. INFOODS will continue to use a dash – for unknown or unspecified or mixed method of determination or for unspecific component while EuroFIR will use the three notations U, UN or UNK.
2. For fatty acids, INFOODS will continue using D before listing the number of carbons while EuroFIR will us ':', e.g. FD20 vs. F:20
3. In INFOODS, conversion factors are regarded as components and always start with X. (**Note**: INFOODS needs to add to some conversion factors for which equivalent they are to be used. For example, XCARTA (= Conversion factor for beta-carotene equivalent of alpha-carotene) can convert alpha-carotene to VITA (retinol equivalent) or to VITA_RAE. The value of XCARTA would be different for the two cases. Therefore two different tagnames are needed. A naming system will have to be investigated). EuroFIR AISBL will not use component identifiers for conversion factors as these are documented as part of the calculation method.
4. EuroFIR will continue using component identifiers and add specific information on methods, expression and definition in different fields. Exceptions to this rule are done for e.g. carbohydrates and fibre. This will continue. INFOODS will continue to publish component identifiers which group components with comparable methods, expressions and definitions.
5. EuroFIR has vitamin equivalents as units and uses a Method Indicator (e.g. "Niacin equivalents calculated from niacin and tryptophan" [MI0421]) indicating how to calculate the niacin equivalent. INFOODS treats vitamin equivalents as component identifiers with metric units where all vitamin equivalents are the sums of the contributing components which are adjusted for their relative vitamin activity by specific conversion factors (e.g. NIAEQ = NIA + TRP/60). EuroFIR AISBL will investigate if they would like to change the use of equivalents as units and have them as component identifiers (like in INFOODS).

6. Both will add Roman letters to minerals to indicate the valence states (e.g. ASIII). Previously, it was decided to use the '+' sign (e.g. AS3+) but this is impossible for INFOODS.

Other issues:

Agreements:

1. INFOODS agreed to add version numbers to their future releases of component identifiers and to add a field with the corresponding EuroFIR component names.
2. Agreement to add components by giving priority to nutrients and bioactive compounds when used in food composition databases. No firm agreement was reached on additives (e.g. cyclamate)
3. It will be up to each compiler to add '_LABEL' for all conversion factors and components in the database for labelling purposes.
4. In the future, Ruth Charrondiere will send new tagnames to the INFOODS mailing list and to the tagname focal points of the INFOODS regional data centres who should collect the opinion of everybody under their responsibility and send them back to Ruth Charrondiere.
5. INFOODS will communicate the tagname naming rules together with new proposals on tagnames (and put them on the web?)

Carbohydrates

The analytical capacity of carbohydrates is not reflected in nutritional terms such as mono-, di-, oligo- and polysaccharides. Also the newly proposed dietary fibre definition and method needs further discussion which goes beyond the time available for this meeting.

Agreement: Naming issues of carbohydrates in general and on oligosaccharides in specific will be discussed in a separate working group comprised of Elizabeth Wenzel, Klaus Englyst, Mariana Santos, Beulah Pretorius and Susanne Westenbrink.

Bioactive compounds

EuroFIR uses numerical codes in eBASIS and INFOODS adds them as they become necessary. It is necessary to find a common naming system.

Agreement: Naming issues of bioactive compounds including flavonoids, antioxidant activity and free vs. bound components will be discussed in a separate working group comprised of Joanne Holden, Elizabeth Wenzel, Barbara Stadlmayr, Jenny Plumb and probably someone from IMNU.

Lipids and fatty acids

Agreements:

1. Both will use C for cis and T for trans. EuroFIR AISBL will investigate if they will continue the use of CIS for cis and TRS for trans in selected cases as they intended to have different meanings.
2. To indicate all trans isomers in *all-trans* polyunsaturated fatty acids, e.g. F18:3TTTN3 or F18D3TTTN3
3. Put always N at the end of the component identifier and all other information before, e.g. F18D1TN2 or F18:1TN2
4. A systematic naming for radicals will be decided between both organizations if the need arises
5. Add component identifiers FAPUC and FAPUT
6. Not distinguish natural from introduced isomers as analytically they can not be differentiated

7. Both will use I for iso and AI for anteiso. The usefulness of ISO by EuroFIR will be investigated (used in USDA?)
8. Outstanding issues will be further discussed in a separate working group comprised of Joanne Holden, Ian Unwin, Mark Roe, T. Longvah, Ruth Charrondiere and Lydia ??

Folate

Folate and folate isomers are clearly defined. A tentative agreement was found on folate isomer naming during e-mail discussion that took place during one year between EuroFIR and INFOODS. Once published, INFOODS is not willing to change naming of component identifiers frequently only because EuroFIR suggests new naming systems. INFOODS urged EuroFIR to keep to the naming once the component identifiers are published by INFOODS.

Agreements:

1. EuroFIR will consider adding FOLDFE from INFOODS
2. EuroFIR will consider adding 'determined by microbiological method' to FOL
3. EuroFIR will consider keeping naming of folate isomers as agreed between both organizations one year ago

There was no time to discuss component grouping or vitamins.

Annex 1

Background to the Joint INFOODS/EuroFIR workshop on Component Identification

Prepared by Ruth Charrondiere and circulated on 13 September 2011 to foreseen participants.

During the last Joint INFOODS/EuroFIR workshop on Component Identification in 2009 in Bangkok the following decisions were taken (some only on a tentative basis) on naming and procedures concerning future collaboration between INFOODS and EuroFIR.

Harmonization process

Previous decisions:

It was agreed that in the future, when EuroFIR or INFOODS have a new set of component identifiers ready for publication, that they should be the same between both organizations (except fatty acids for the colon vs. D, components determined with empirical methods and unspecified components, conversion factors). This means that after finalisation of internal discussions on new component identifiers within each organization, but prior to their publication, the two organizations will prepare a list of the new component identifiers (new and updated ones) and send it to the other organization with the objective to agree as much as possible on a common set of component identifiers.

General issues including naming and additions

Previous decisions:

7. INFOODS will continue to use a dash – for unknown or unspecified or mixed method of determination while EuroFIR will use the three notations U, UN or UNK.
8. In INFOODS, conversion factors are regarded as components and always start with X.
9. EuroFIR uses A Method Indicator (e.g. “Niacin equivalents calculated from niacin and tryptophan” [MI0421]) indicating how to calculate the niacin equivalent. INFOODS treats them as component identifiers with metric units and where all vitamin equivalents are the sums of the contributing components which are adjusted for their relative vitamin activity by specific conversion factors (e.g. NIAEQ = NIA + TRP/60).
10. agreement to add mineral with valence states, e.g. AS3+
11. INFOODS agreed to add version numbers to their future releases of component identifiers and to add a field with the corresponding EuroFIR component names.
12. Agreement to add only those components which are used in food composition and/or are determined separately for food composition purposes. No firm agreement was reached on additives (e.g. cyclamate)
13. It was suggested to add ‘_LABEL’ for all conversion factors and components in the database for labelling purposes. However, this requires further discussions.
14. Different component names were discussed and harmonization reached in most cases

INFOODS has worked on a set of new tagnames but has not released them yet (to be done until the end of 2011)

Lipid components

Previous decisions:

Because the INFOODS system is conceived to use component identifiers as mark-up language tags in electronic data interchange, the use of colon is prohibited. EuroFIR uses the component identifiers as attributes in data interchange and is therefore free to use the colon in their component identifiers. This is done in fatty acids, e.g. lauric acid has the component identifiers F12:0 in EuroFIR and F12D0 in INFOODS.

Tentative agreements reached:

- Both organizations will use only uppercase letters

- For the cis/trans isomers, both organizations will:
    - use C and T (not Z and E);
    - put C for cis or T for trans in front of double bond position counting from the COOH end, if it is known where they occur;
    - put at the end of the component identifier either a single T if at least one double bond is trans or a single C if it is known that all double bonds are cis isomers;
    - identify unknown positions of known cis/trans isomers by putting at the end of component identifier as many C and T as double bonds while putting C first followed by T, e.g. CCT if two cis isomers and one trans exist without knowing their position;
    - for individual fatty acids with unknown cis/trans isomers, both INFOODS and EuroFIR will not add any specific sign, e.g. F16D2 or F16:2, respectively;.
    - for fatty acids with unknown number of double bounds, INFOODS will not add any sign and EuroFIR UN for unidentified, e.g. F16 vs. F16:UN
    - for the sum of polyunsaturated fatty acids (FAPU), it is recommended to create new component identifiers in both systems to indicate cis/trans fatty acids (e.g. FAPUC and FAPUT) and promote their use.
- iso/anteiso: I and AI
- for sums of fatty acids, additional info on which fatty acids are included should be added

Agreement still needed:

- radical naming
- natural vs. introduced trans isomers through hydrogenation

Outstanding questions

- why is iso sometimes I and sometimes ISO, e.g. F17:0I and F18:2ISO
- why is trans sometimes TRS and sometimes T, and cis sometimes CIS and sometimes C (new question)

EuroFIR new propositions (from http://www.eurofir.eu/content/compthes/fa_identifiers as of 28.7.2011)

Fatty acids are specified using the common convention F*x*:*y* where *x* is the number of carbon atoms and *y* is the number of unsaturated C=C bonds. For branched-chain fatty acids, the number *x* is the total number of carbons and thus, for example, the isomer F15:0I is13-methyltetradecanoic acid, systematically named as a C_{14} compound.

n-Notation and monounsaturated fatty acids

In nutritional contexts, the position of double bonds in unsaturated fatty acids is commonly specified using *n*-notation shorthand, which counts from the methyl end of the chain. The system is widely used in the Thesaurus for fatty acid descriptors and identifiers. However, its scope has strict limitations, which the book Food lipids (pp 8-9) states as:

Shorthand nomenclature cannot be used for fatty acids with trans or acetylenic bonds, for those with additional functional groups (branched, hydroxy, etc.), or for double bond systems (2 or more double bonds) that are not methylene interrupted ([i.e. that are not] isolated or conjugated).

Wider usage of *n*-notation for fatty acid identifiers depends on extra information provided before the shorthand notation, which must always terminate the identifier. Configuration is shown explicitly, for example F16:1CN7 is used for palmitoleic acid and F16:1TN7 for its trans isomer palmitelaidic acid. Although rarely occurring, substitution needs to be considered and should be recorded specifically. The current identifier for ricinoleic acid (12-hydroxy-*cis*-9-octadecenoic acid) is F18:1N9O, which would be better as F18:1O12CN9. This would distinguish it from the *trans* form ricinelaidic acid, as well as accommodating any alternative locations of the hydroxy group.

Polyunsaturated fatty acids

Polyunsaturated fatty acids provide further complications as the positions and configurations of the several double bonds must be specified unambiguously. The termination CN*x* is used to indicate strict *n*-notation, i.e.the methylene separated (=CH-CH_2-CH=), all-*cis* form; for example gamma-linolenic acid is F18:3CN6. However, because the term *trans*-fatty acid is used when one or more bonds is *trans*, the explicit identifier F18:3TTTN3 is used for the all-*trans* structure linolenelaidic acid. The

F18:3TN3 would be used for the total of n-3 *trans* isomers, whereas overall *cis* or *trans* totals for a fatty acid are indicated by the 3-letter terminations CIS or TRS, e.g. F18:3TRS for total *trans*-octadecatrienoic acids.

Conjugated fatty acids

The total of conjugated forms for a fatty acid use the 3-letter terminator CON; at present only F18:2CON is defined. Where specific positional information is included, this is done using the chemical convention of counting from the functional group, i.e. the carboxylate end. Thus F18:2C9T11 is defined for rumenic acid (9-*cis*,11-*trans*-octadecadienoic acid) and F18:2T10C12 for the other most common isomer. However, these may co-occur with the 9-*cis*,11-*cis* and 10-*cis*,12-*cis* isomers, so it may be necessary to identify further isomers and mixtures of them.

Totals, remainders and unidentifieds

A wide range of terms is available for reporting totals of fatty acids and of their isomers. Some summate isomers of mono- and polyunsaturated acids, e.g. *fatty acids, total n-3* [FAN3] and *fatty acids, total cis n-3* [FACN3]. Others represent totals within the different types of fatty acid, e.g. *fatty acids, polyunsaturated, total n-3* [FAPUN3]. This overall total has more specific related totals, e.g. for the (all-)*cis* isomers [FAPUCN3], the long-chain acids [FAPUN3LC] and fatty acids derived from particular food sources such as fish [FAPUN3FI].
Terms are included for various remainders and "others". The one term now using "other" is *fatty acids, polyunsaturated, other (= PUFA-linoleic-linolenic)* [FAPUOT] and thus it specifically defines the fatty acids that are included (except that it does not state clearly whether both alpha- and gamma-linolenic acid are included).

For discussions of component identifiers for fatty acids that are requested for inclusion in the Component Thesaurus, see the topic Fatty acid coverage.

Carbohydrates and fibre

Previous decisions:
INFOODS will have different tagnames for empirical methods (e.g. for different fibre methods) and different expressions (e.g. in monosaccharide equivalents, total vs. available carbohydrates) while in general EuroFIR will not (even there are some exceptions to this rule)

Component grouping

The grouping of components was not discussed because of limited time.
For this meeting, INFOODS send a draft proposal for discussion (see annex 1)
EuroFIR

Folate

Previous decisions as tentative agreements:
- FOLAC: folic acid (EuroFIR will replace FOLACID)
- FOLCH3H4: 5-Methyltetrahydrofolate (EuroFIR and INFOODS will change)
- FOLHCOH4: 5-Formyltetrahydrofolate (EuroFIR and INFOODS will change)
- FOLCH3H2: 5-methyl-dihydrofolic acid (EuroFIR and INFOODS will change)
- FOLHCO10H4: 10-formyldihydrofolate (EuroFIR and INFOODS will change)
- FOLHCO10: 10- formylfolic acid (EuroFIR and INFOODS will change)
- FOLSUM: folate, sum of vitamers, determined by HPLC (EuroFIR will add)
- FOLFRE: folate, free/unconjungated (new scope note)

EuroFIR new propositions (from http://www.eurofir.eu/content/compthes/folates as of 26.7.2011)
Discussion of folates within the Component Thesaurus can be based on the updates and policy issues described in the report for version 1.1, with a minor revision in version 1.2. These descriptions are available in the attached document .

Mode of expression

Compositional values for individual folates and folate totals should be expressed as monoglutamates. The term *dietary folate equivalents* is not required in the EuroFIR thesauri, either as a component identifier or as a unit, as it is represented by the code FOL (*folate, total*) plus the method indicator MI0453 (*Folate by factored calculation from intrinsic folic acid and added folic acid*).

Conventions for identifiers

All codes for folate component start with the letters FOL Uninverted forms such as THF for tetrahydrofolate are avoided as these make codes hard to find in an alphabetical listing, as well as being potentially ambiguous with other acronyms widely used in chemistry (e.g. THF = tetrahydrofuran).
The next structural detail specified is the level of saturation, with dihydrofolates and tetrahydrofolates having codes beginning FOLH2 and FOLH4, respectively. Then any substitution is indicated using a two-letter representation of the substituent, followed by its locant. The substituted folates currently in the thesaurus are 10-formyldihydrofolate [FOLH2FM10], 10-formylfolic acid [FOLFM10], 5-formyltetrahydrofolic acid [FOLH4FM5], 5-methyldihydrofolic acid [FOLH2ME5] and 5-methyltetrahydrofolate [FOLH4ME5].

Conjugated and bound folates

A conjugated folate has a polyglutamate moiety usually consisting of 2 to 6 glutamic acid residues. Bound folates are mono- or polyglutamates bound to proteins, etc. The component terms for "folate, bound" [FOLB] and "folate, free" [FOLFRE] have been inactivated as they are incompatible with the expression of values as monoglutamate.

Synthetic folic acid

The term for "folic acid" (i.e. pteroylmonoglutamic acid) is compatible with the standard mode of expression, but is specific to synthetic folic acid used to fortify foods. This form is considered to be more active than intrinsic (i.e. naturally occurring) folate and thus its compositional value in a fortified food is necessary information for the calculation of the *total folate* value. For version 1.1 of the thesaurus, 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.

Mixtures and condensed products

INFOODS new propositions

- as INFOODS can only use ‘-’ and ‘_’ to use ‘_’ for sums, e.g. CYS_MET for CYS+MET or F16D1N7_F16D1N9 for FA 16:1 n-7 + FA 16:1 n-9

EuroFIR new propositions (from http://www.eurofir.eu/content/compthes/mixtures as of 16.8.2011)

- use of ‘+’ between components "A+B", e.g. LUTN+ZEA or F14:1CIS+F16:1CIS+F18:1CIS

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 can 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. Use of 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

A condensation products results when two or more moieties combine to form a single molecule, accompanied by the loss of small molecules, often water. Food components that can be considered as condensation products include esters, other types of glyceride, and higher sugars. Their constituent parts may already be 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 problems of ambiguity in a code such as RETOLLIN. It should be discussed for introduction when version 2.0 of the Component Thesaurus is implemented.

(**Annex 1 of the background document)**

Draft INFOODS proposition of components

group	Description
01	General description of food
02	Macronutrients including energy
021	Energy
022	Protein
0221	Amino acids: individual and aggregations
0222	Nitrogen and protein expressions, conversion factors
0223	Protein components
0224	Other nitrogen-containing components
0225	Protein quality
023	Fat, fatty acids, fatty acid conversion factor
0231	Fatty acids
0232	Fat components
0233	Phospholipids
0234	Fat quality
024	Carbohydrates, carbohydrate fractions
0241	Sugars
02411	Monosaccharides
02412	Disaccharides
0242	Oligosaccharides
0243	Polysaccharides
02431	Dietary fibre, fibre, dietary fibre fractions
024311	Dietary fibre fractions
025	Water
026	Alcohols
027	Ash and other solids
028	Polyols
029	Organic acids
03	Minerals
033	Heavy metals/ contaminants
034	Other minerals
04	Vitamins
041	Fat soluble vitamins
0411	Vitamin A, retinol
0412	Carotenoids
0413	Vitamin D
0414	Vitamin E
0415	Vitamin K
042	Water soluble vitamins
0421	Thiamin (vitamin B1)
0422	Riboflavin (vitamin B2)
0423	Folate

0424	Niacin
0425	Pantothenic acid
0426	Vitamin B6
0427	Vitamin B12
0428	Biotin
0429	Vitamin C
05	Sterols
051	Plant sterols
052	Cholesterol
06	Bioactive compounds
061	Flavonoids
0611	Flavanols/flavans
0612	Flavonones
0613	Flavones
0614	Flavonols
0615	Isoflavonoids/isoflavones
062	Tannins
063	Phenolic acids
064	Other bioactive compounds
065	Antioxidant activities
07	Biogenic amines
08	Purines
09	Additives
10	Choline and derivates
11	?? Not knowing where to classify
12	Miscellaneous