IFRA Natural Complex Substances (NCS) TF procedure to derive compositional data for NCS
(Revision 1 Final June 23, 2021)

Objective
The main objective of the IFRA NCS TF is to maintain up to date the IFRA/IOFI NCS Complex Ingredient Constituent Compendium (CICC), formerly called the 'IFRA-IOFI NCS matrix', to ensure consistency and harmonization on NCS characterization with regard to constituents to allow for sameness check and related activities under various IFRA, IOFI and RIFM activities:
•   IFRA Standards, including the update of Annex I on contributions from other sources,
•   IFRA/IOFI Labelling Manual,
•   RIFM Database,
•   RIFM Safety Assessments.

NCS TF Structure, Set up and Membership
The NCS TF builds on the expert knowledge of its members. It is open to all members of IFRA (direct members, members of National association or supporting members) if they can contribute by providing knowledge on the composition of NCS used in the Fragrance and Flavor industry.

The current membership includes experts from (in alphabetical order):
Berje, Firmenich, Givaudan, I.F.F., Kerry, Mane, Robertet, Symrise and Ultra International

Further, the membership includes representatives from related trade associations including EFEO, FEMA, IOFI as well as RIFM. Further, RIFM members may be admitted to the group if they commit to the IFRA Code of Practice for the fragrance activities they have that are covered by the IFRA Standards and can clearly contribute knowledge on the composition of NCS used in the Fragrance and Flavor industry.

Collecting and processing of data in the TF
The data established by the TF are based on several sources, including REACH dossiers, reliable literature data and individual information from the above-mentioned members of the NCS TF and other members of IFRA (in case they use the respective NCS quality under review and have compositional information). All data are reviewed during regular conference calls.

The aim of the review during the conference call is to ensure that the data are consistent and that there are no outliers. In some specific cases, this can lead to the deletion/modification of the concentration of a constituent entered by one company, the exclusion of the literature data when significantly deviating from industry quality or the request for verification of data as an action.

The way the review is organized leads to 'typical' values, and not mean values based on a large number of analytical data coming from several batches. Due to the low number of datapoints it is not possible to provide percentage information sufficiently robust from a statistical point of view.

If relevant differences are recognized between the NCS TF member contributions as well as by comparing with relevant literature information, it is then important to check the analytical method applied in relationship with the quantification approach giving the typical value.

The NCS TF aims at ensuring that the typical values provided via the CICC are aligned as much as possible with the composition data published elsewhere (e.g., FEMA publications, REACH dossiers).

The TF tries to provide compositional data of the whole NCS, not just the volatile part. Therefore information about the non volatiles is also collected, and often based on literature data.

Adding up typical composition values in some cases may exceed 100% if added up for all components, which can be explained by batch variations. If normalization is required, the percentages are adjusted by taking the average individual component %, divide by total concentration times 100. E.g. if total concentration is 105, and linalool is present at 1% in 105, this is normalized 1/105*100 = 0.95%.

History and agreements when starting to support the compositional network

Before 2017, a consultant highly experienced in NCS (David Moyler, Moyler Consultancy) was maintaining up to date the IFRA/IOFI NCS matrix. He was progressively including all the changes arising from discussion topics with the IFRA NCS TF and the IFRA-IOFI GHS TF and new or revised data as from the literature. He further categorized the NCS composition depending on the reliability of the source of the composition data with a Data Reliability Factor (DRF), DRF1 being the most reliable, down to DRF4.

The definitions are as follows:

DRF1, Reliable without restriction

Collaborative studies by several laboratories on many authenticated NCS, resulting in statistically analyzed compositions by GC-MS analysis. Representative for DRF1 data would be the work of the EFFA REACH task force in which many trade laboratories contributed multiple analysis results, using a standardized template of constituents.

DRF2, Reliable with restriction

Collaborative study by several laboratories on one authenticated NCS sample, under standardized, calibrated procedures. Representative of DRF 2 data would be the published work of the Royal Society of Chemistry essential oil analysis group, who studied typical individual pure oils of given batch provenance, provided by the BEOA (British Essential Oil Association).

DRF3, Not reliable:

Studies or data from peer reviewed published literature, supported by an ISO standard, Pharmacopeia or Council of Europe specification. However, this data, often missing a complete description of the NCS composition, may be helpful for supporting a 'weight of evidence approach'.

DRF4, Not assignable:

Studies or data from literature, which do not give sufficient experimental details and may only be listed in abstracts or secondary literature like books or reviews. It may be based on a compositional calculation from the essential oil (and marked as such) for terpenes, concretes or absolutes containing resins or fatty acid esters of characterized type. However, this data may be helpful for supporting a 'weight of evidence approach'.

Considerations for the scope of the work of the NCS TF

In 2017 the NCS TF officially took over the task of establishing the compositional data of NCS and on establishing "typical values" for such NCS, as described above.

With the request from RIFM to provide compositional information for several hundred NCS in the scope of the RIFM NCS SA program, some pragmatic decisions were taken to be able to administer the task.

Due to the sense of urgency of the RIFM request, the IFRA NCS TF is performing the review as follows: NCS for which DRF is 1 or 2 – the IFRA NCS TF considers there is enough confidence on the reliability of the composition data of these NCS . There is thus no further work needed on these NCS at the moment , unless there are questions raised that would need to be addressed.

DRF1 and 2 data might undergo occasional spot checking when used in draft NCS SA by dedicated members of the NCS TF.

Highest priority for establishing reliable compositional data is therefore given to NCS for which DRF is 3 or 4 as most of these NCS represent low volumes of use with low representativity in the market and the reliability of available compositional data is therefore questionable.

Besides contributing to the establishment of the composition information the NCS TF also provides input and advice on adequate material description including but not limited to CAS-numbers or ISO-code.

Materials out of scope of the NCS TF work

There are a number of NCS for which the TF will not be in a position to establish a typical composition. Those are either based on starting material of similar but variable origins (oil made of different types of citrus fruits for example) or derived by individual, non-standardized 'in house' processes that may vary from producer to producer or even a combination of both factors. The table below lists NCS out of the scope of the NCS TF

Type of NCS	Iso Code	Process Description		Reason
concentrated essential oil	2.6	essential oil treated by a physical process in order to concentrate one or more components	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
Distillate	2.8	product of condensation obtained after distillation of a natural raw material	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
extract	2.13	product obtained by treating a natural raw material with one or several solvents	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
exudate	2.14	Natural raw material excreted by plant	No	Part of vegetal
Gum	2.15	Similar to exudate	No	Part of vegetal
Gum Oleoresine	2.16	Similar to exudate	No	Part of vegetal
Gum Resin	2.17	Similar to exudate	No	Part of vegetal

Natural Raw Material	2.19	natural raw material of vegetal, animal or microbiological origin, as such, obtained by physical, enzymatic or microbiological processes, or obtained by traditional preparation processes (e.g. extraction, distillation, heating, torrefaction, fermentation)	No	General definition of raw material. Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
non-concentrated extract	2.20	product obtained by treating a natural raw material with one or several non-eliminated solvents	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
rectified essential oil	2.24	essential oil (2.11) which has been subjected to a fractional distillation in order to modify the content of certain compounds and/or its color	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
"terpeneless and sesquiterpeneless" essential oil	2.28	rectified essential oil from which certain fractions containing mainly the mono- and sesquiterpene hydrocarbons have been partly eliminated	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
"terpeneless" essential oil	2.29	rectified essential oil (2.24) from which certain fractions containing mainly the monoterpene hydrocarbons have been partly eliminated	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
Terpenes	2.30	products mainly consisting of terpenic hydrocarbons obtained as by-products of an essential oil by distillation, concentration or other separation techniques	No*	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.
"x-free" essential oil	2.33	essential oil from which a component "x" has been partly or completely eliminated	No	Refers to 'in house' processes that may vary from producer to producer. IFRA NCS TF cannot provide a typical concentration profile for the NCS.

*Decision on a case-by-case basis, e.g. 'No' for Citrus terpenes spp but 'Yes' for defined species like Mandarin