

# Setting the scene – Regulatory Expectations

Concawe Workshop

8 November 2023

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# Annex VI Section 2 - Composition of a substance

- 2.3.2. Names of constituents and impurities
- In the case of a substance of unknown or variable composition, complex reaction products or biological materials (UVCB):
  - names of constituents present at a concentration of  $\geq 10\%$ ;
  - names of known constituents present at a concentration of  $< 10\%$ ;
  - for constituents that cannot be identified individually, description of groups of constituents based on chemical nature;
  - description of the origin or source and the manufacturing process
- 2.3.3. Typical concentration and concentration range (in percentage) of constituents, groups of constituents that cannot be identified individually and impurities as specified in point 2.3.2

## Annex VI Section 2 – Analytical information

- 2.3.5. All necessary qualitative analytical data specific for the identification of the substance, such as ultra-violet, infra-red, nuclear magnetic resonance, mass spectrum or diffraction data
- 2.3.6. All necessary quantitative analytical data specific for the identification of the substance, such as chromatographic, titrimetric, elemental analysis or diffraction data

## Annex VI Section 2 – Analytical information

- 2.3.7. Description of the analytical methods or the appropriate bibliographical references that are necessary for the identification of the substance (including the identification and quantification of its constituents and, where appropriate, its impurities and additives). The description shall consist of the experimental protocols followed and the relevant interpretation of the results reported under points 2.3.1 to 2.3.6. This information shall be sufficient to allow the methods to be reproduced

## Annex XI Section 1.5 – Structural similarity for UVCB substances

- *Structural similarity for UVCB substances shall be established on the basis of similarities in the structures of the constituents, together with the concentration of these constituents and variability in the concentration of these constituents. If it can be demonstrated that the identification of all individual constituents is not technically possible or impractical, the structural similarity may be demonstrated by other means, to enable a quantitative and qualitative comparison of the actual composition between substances.*

# Annex XI - Structural similarity for UVCB substances

- **Structural similarity is a prerequisite for read-across**
- Establishing structural similarity for UVCB substances
  - Identification of constituents and their concentrations
  - Variability in concentration of constituents

# Annex XI - Structural similarity for UVCB substances

- By understanding dis-/similarities in structures of constituents
- Structures are the same/similar/not
  - Concentrations are similar vs. different
  - Variation of concentrations is similar vs. not

## Annex XIII - PBT assessment

- **Annex XIII:** The identification shall also take account of the PBT/vPvB-properties of relevant constituents of a substance
- R11 guidance – *Regardless of whether full substance identification is possible or not for the whole composition, the registrant should make efforts for carrying out a PBT/vPvB assessment for all constituents, impurities and additives present in concentrations above 0.1% (w/w). Section R.11.4.2.2 provides further insight into how to carry out PBT/vPvB assessment for fractions of the substance that cannot be fully identified by the registrant*



# Composition – detail and context

- Linear alkanes (n-alkanes)
- Branched alkanes (iso-alkanes)
- Cyclic alkanes (Naphthenics)
  - Mono-cyclic
  - Di-cyclic
  - Tri-cyclic
  - Tetra-cyclic
- Aromatics
  - Mono-aromatics
  - Di-Aromatics
  - Tri-aromatics
  - Tetra-aromatics
- Aromatics-Naphthenics
  - Mono-aromatics-Naphtenics
  - Di-aromatics-Naphthenics

Information on carbon number range for each class. Concentration (typical) and concentration ranges for each reported constituent (group of constituents).

Additional information, e.g. PAHs

# Thank you

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