How to bring your registration dossier in compliance with REACH – Tips and Hints (Part 3)

Multi constituent and UVCB substances

14th May 2013

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Multi constituent and UVCB substances

- Substances with several chemically defined constituents > 10% m/m
- None of the constituents appear at a concentration >= 80% m/m

- Substances with many well-defined constituents of variable concentrations
- Substances with many not well-defined constituents
- Substances of defined biological origin
- Described by educts and process

Partition Coefficient Octanol-Water (log K_{ow})

- Describes the distribution of the substance between two phases (octanol and water) in close contact to each other
- Required for the exposure and risk assessment:
  - Environmental distribution
  - Bioaccumulation potential (PBT-assessment)
- Annex VII 7.8. requirement

log K_{ow} and UVCB substances

- **HPLC method** is generally the preferred method for UVCB substances (EU A6, OECD 117).
- log K_{ow} ranges can be provided for UVCB substances, but:
  - Ranges have to be **concrete and narrow** to be able to reflect their significance in the risk assessment.
  - Multiple values may describe the properties of the substance better if **groups of constituents** can be separated by HPLC.
  - An indication of the **proportion of the substance** covered by a value or a range of value should be provided.
- The slow-stirring method (OECD 123) and the shake flask method in combination with **chromatographic analysis may be used** to describe the properties of the substance.

$logK_{ow}$ and multi constituent substances

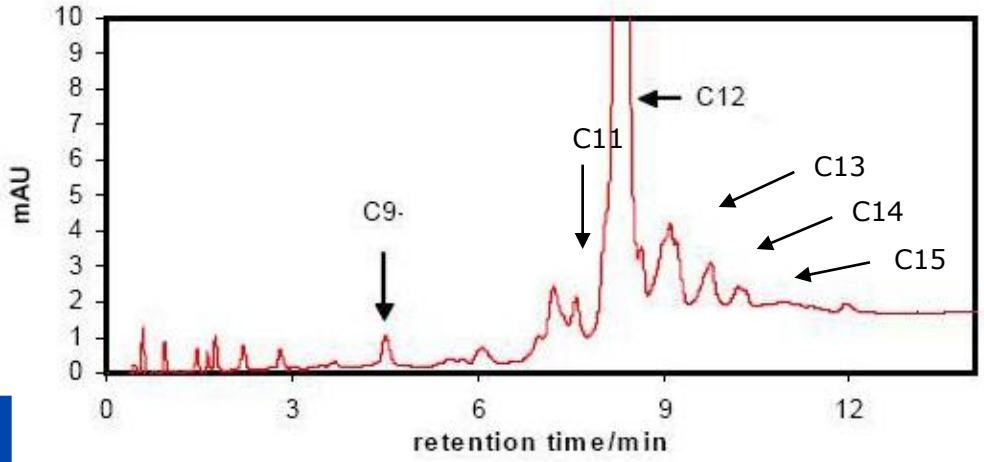
- The approach for UVCBs can be used, and

- In the case of **well defined constituents**: a value for each individual constituent using an individual endpoint study record in IUCLID may be provided

Example logK_{ow}:

Constituent	Octanol (conc.)	Water (conc.)	Log Kow
C9	1 000 000	1 000	3
C11	5 000 000	500	4
C12	10 000 000	100	5
C13	50 000 000	50	6
C14	100 000 000	10	7
C15	500 000 000	5	8

Slow-Stirring Study



HPLC chromatogram of n-octanol phase from slow-stirring method

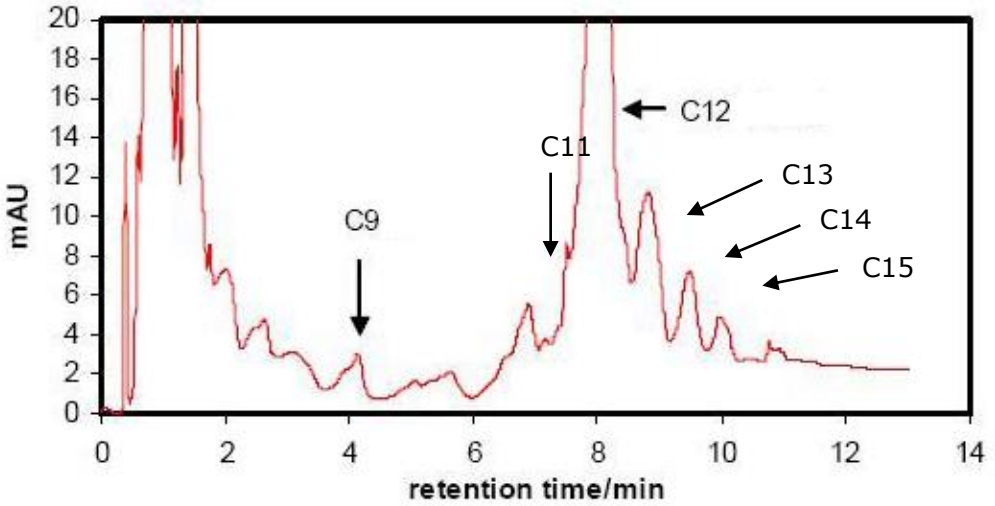
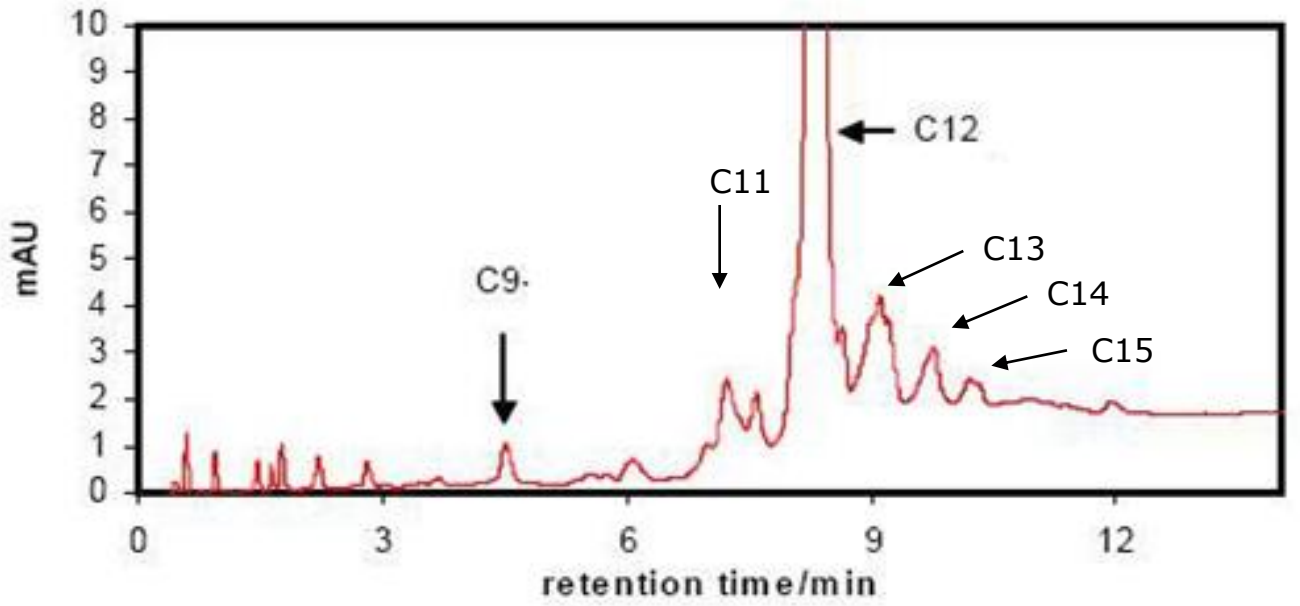


Figure 2. HPLC chromatogram of water phase from slow-stirring method

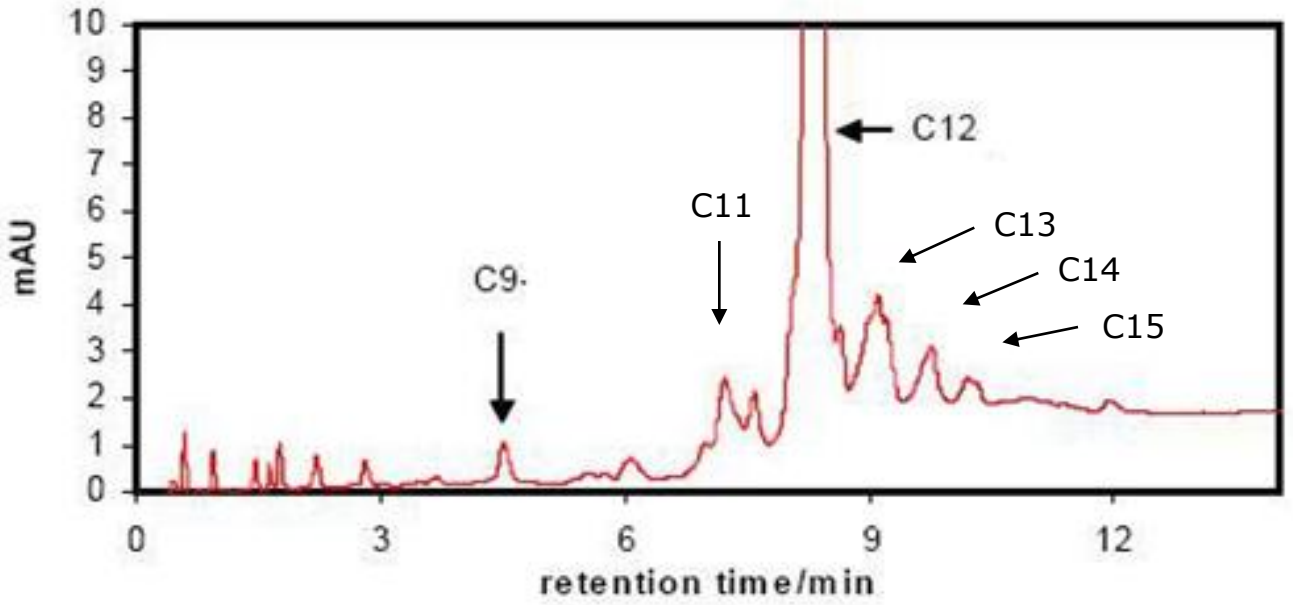
Water solubility

Constituent	WS [mg/l]
C9	8
C11	17
C12	600
C13	50
C14	40
C15	20



Dissociation constant

Constituent	pKa
C9	5.3
C11	5.8
C12	6.5
C13	6.9
C14	7.7
C15	8.0



http://echa.europa.eu/documents/10162/13632/information_requirements_r7a_en.pdf

Thank you