

## **Substance Identification of MeCI**

## Analytical proof of identity & composition of the substance according to Annex VI of the REACH regulation:

- NMR: <sup>1</sup>H & <sup>13</sup>C-NMR in solution (optional instead of GC-MS)
- UV-VIS & IR: as gas
- HPLC: waiver
- GC-MS: provides identity and quantitative composition of substance incl. impurities.

Test preferably according to published standards, otherwise to validated lab methods.

REACH regulation 1907/2006, Annex VI, 2:

2. IDENTIFICATION OF THE SUBSTANCE

For each substance, the information given in this section shall be sufficient to enable each substance to be identified.

If it is not technically possible or if it does not appear scientifically necessary to give information on one or more of the items below, the reasons shall be clearly stated.

- 2.1. Name or other identifier of each substance
- 2.1.1. Name(s) in the IUPAC nomenclature or other international chemical name(s)
- 2.1.2. Other names (usual name, trade name, abbreviation)
- 2.1.3. EINECS or ELINCs number (if available and appropriate)
- 2.1.4. CAS name and CAS number (if available)
- 2.1.5. Other identity code (if available)
- 2.2. Information related to molecular and structural formula of each substance
- 2.2.1. Molecular and structural formula (including SMILES notation, if available)
- 2.2.2. Information on optical activity and typical ratio of (stereo) isomers (if applicable and appropriate)
- 2.2.3. Molecular weight or molecular weight range
- 2.3. Composition of each substance
- 2.3.1. Degree of purity (%)
- 2.3.2. Nature of impurities, including isomers and by-products
- 2.3.3. Percentage of (significant) main impurities
- 2.3.4. Nature and order of magnitude (... ppm, ... %) of any additives (e.g. stabilising agents or inhibitors)
- 2.3.5. Spectral data (ultra-violet, infra-red, nuclear magnetic resonance or mass spectrum)
- 2.3.6. High-pressure liquid chromatogram, gas chromatogram

2.3.7. Description of the analytical methods or the appropriate bibliographical references for the identification of the substance and, where appropriate, for the identification of impurities and additives. This information shall be sufficient to allow the methods to be reproduced.