Infochemical effects of repellents (PT 19 biocides) in surface waters: suitable test substances for proof of concept

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Introduction
The environmental relevance of infochemical effects has been hypothesized, but is not yet confirmed by experimental observations. This project contributes a selection of suitable test substances as the first step of systematic investigations on the impact of potential anthropogenic infochemicals with regard to the chemical communication of biota in freshwater.

Repellents (PT 19 biocides) and odorants are likely candidates that may affect the behaviour of aquatic populations and communities. The mostly polar and stable compounds may disturb the chemical communication between organisms and may cause effects like organismic drift (downstream dislocation of e.g. crustaceans and insect larvae in streams). Most emissions of repellents to surface waters occur indirectly via waste waters and sewage treatment plants or directly in bathing water (washing off skin and clothes).

Objectives
- Identify substances with a realistic infochemical potential
  - Repellents and attractants (Biocides Directive 98/8/EC)
  - Natural infochemicals, e.g. alarm substances, pheromones
  - Anthropogenic chemicals, e.g. odorants, cosmetic ingredients, pesticides, pharmaceuticals, industrial chemicals
- Assess their relevance to aquatic compartments
  - Discharge into surface waters
  - Environmental monitoring
  - Use in consumer products
- Prefer substances with minor direct toxicities at low dose
  - Foreseeable avoidance reactions shall not overrule the infochemical effects.
- Consider physico-chemical liability for testing
  - Water solubility >1 mg/L
  - Medium lipophilicity (log Kow <4)
  - Stability (hydrolysis, biodegradation)

Results
In this literature study suitable chemicals were selected for confirmatory assessments of infochemical effects by later laboratory tests. The use patterns and physico-chemical properties of the substances, in combination with limited biological degradability, may indicate potential aquatic relevance with possible chronic impact caused by disturbed aquatic communication.

After due consideration of advantages and limitations, three PT 19 repellents appear suitable test compounds for proof of concept in a subsequent experimental project:
- DEET (CAS 134-62-3),
- Icaridine (CAS 119515-38-7) and
- EBAAP (CAS 52304-36-6).

Another promising candidate for infochemical effects is isophorone (CAS 78-59-1), a natural attractant and an anthropogenic HPV (High Production Volume) solvent.

References
Nendza M, Klaschka U: Wirkungsrelevanz von Repellentien (Produktart 19) und anderen Infochemikalien für Nichtzielorganismen in Oberflächengewässern, Teil II: Laborstudie. FKZ 3712 67 417.2

Infochemical effects
Most organisms live in an odour environment and recognize their biotic and abiotic surroundings via sophisticated, specific and dynamic blends of odorants, called infochemicals. The infochemicals are major means of communication in aquatic ecosystems, because other senses, e.g. vision, are less efficient in natural, often turbid waters.

Clouds of odours from various sources, as visualized by the photograph of coloured ink, can overlap and influence each other.

The infochemical effect is defined as the manipulation of smell perception in organisms by anthropogenic substances which may result in ecologically relevant behavioural disorders.

Procedure
Stepwise approach to identify suitable test substances for proof of concept regarding infochemical effects in surface waters:

<table>
<thead>
<tr>
<th>Potential infochemical effect</th>
<th>Odorant</th>
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<tbody>
<tr>
<td>31 potential candidates</td>
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<tr>
<th>Relevance for the aquatic compartment</th>
<th>Physico-chemical properties (volatility, solubility)</th>
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<th>Persistence</th>
<th>Aquatic toxicity</th>
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<th>Commercial availability</th>
<th>Use pattern</th>
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<td>Analytical determinability</td>
<td>PEC/PNEC</td>
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<tr>
<td>Data availability</td>
<td>3 candidates</td>
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</tbody>
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Suitable test substances for proof of concept
Chemical structures and CAS-numbers of candidate substances for the experimental assessment of infochemical effects:

Conclusions
Four chemicals were selected with the expectation that they may be suitable candidates for the experimental proof of concept of infochemical effects in the subsequent project part. The experimental results may then help to answer the question if there are reasons for concern regarding infochemical effects of PT 19 biocides and other odorants in aquatic ecosystems.

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