

Determination of 4-nonylphenol in water samples using 4-(2,6-dimethylhept-3-yl)phenol as new internal standard

Fischer A.R., Lan N.T.P., Wiedemann C., Heide P., Werner P., Schmidt A.W., Theumer G., Knolker H.-J.
Institute of Waste Management and Contaminated Site Treatment, Technische Universität Dresden,
Pratzschwitzer Str. 15, D-01796 Pirna, Germany; Hanoi University of Science, 334 Nguyen Trai, Hanoi,
Viet Nam; Department of Chemistry, Technische Universität Dresden, Bergstr. 66, D-01069 Dresden,
Germany

Abstract: A new method for determining the endocrine disrupting substance 4-nonylphenol (technical grade=mixture of isomers, 4-NP) from water samples has been developed by using 4-(2,6-dimethylhept-3-yl)phenol (4-sec-NP) as model compound. This branched monoalkylphenol is shown to serve as internal standard (IS) for the determination of technical 4-nonylphenol. To the best of our knowledge, 4-(2,6-dimethylhept-3-yl)phenol (racemic mixture) is a newly synthesized 4-nonylphenol isomer and has not been described elsewhere. Recoveries have been determined by analyzing spiked water samples from distilled water, river water and wastewater. Following acetylation, the compounds were enriched via solid phase extraction (SPE). Analyses of the compounds were performed by capillary column gas chromatography/mass spectrometry (GC/MS), operating in selected ion-monitoring (SIM) mode. The recovery of technical 4-NP using either the newly prepared 4-sec-NP or 4-n-nonylphenol (4-n-NP) as IS have been compared. 4-sec-NP showed slightly better results. However, in the first series of experiments using wastewater, the yields for the derivatization of the two standard compounds were remarkably different. The yield for derivatization of 4-n-NP was approximately 20%, probably due to the difficult matrix of the wastewater. In contrast, the yield for the derivatization of 4-sec-NP was considerably higher (approximately 63%). This problem can be solved by increasing the concentration of the reagent used for derivatization. For better control of the clean-up process, we recommend application of 4-sec-NP as internal standard, at least in water samples with complex matrices (e.g., high content of hydroxylated compounds). © 2010 Elsevier B.V.

Author Keywords: Gas chromatography-mass spectrometry; Internal standard; Nonylphenol isomers

Index Keywords: 4-n-Nonylphenol; 4-Nonylphenol; 4-Nonylphenol isomer; Capillary columns; Complex matrices; Derivatizations; Distilled water; Gas chromatography-mass spectrometry; High-content; Internal standards; matrix; Model compound; Nonylphenol isomers; Racemic mixtures; River water; Solid-phase extraction; Spiked water samples; Water samples; Acetylation; Gas chromatography; Isomers; Mass spectrometry; Phenols; Recovery; Standards; Wastewater; Water content; Extraction; 4 (2,6 dimethylhept 3 yl)phenol; 4 nonylphenol; phenol; river water; unclassified drug; 4-nonylphenol; phenol derivative; acetylation; article; calculation; calibration; capillary gas chromatography; chemical analysis; chemical structure; controlled study; derivatization; intermethod comparison; isomer; mass spectrometry; priority journal; solid phase extraction; surface property; synthesis; waste water; water analysis; water sampling; mass fragmentography; methodology; standard; water pollutant; Gas Chromatography-Mass Spectrometry; Phenols; Reference Standards; Water Pollutants, Chemical

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Correspondence Address: Fischer, A.R.; Institute of Waste Management and Contaminated Site Treatment, Technische Universität Dresden, Pratzschwitzer Str. 15, D-01796 Pirna, Germany; email: axel_rene.fischer@tu-dresden.de

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Authors with affiliations:

- Fischer, A.R., Institute of Waste Management and Contaminated Site Treatment, Technische Universität Dresden, Pratzschwitzer Str. 15, D-01796 Pirna, Germany
- Lan, N.T.P., Hanoi University of Science, 334 Nguyen Trai, Hanoi, Viet Nam
- Wiedemann, C., Institute of Waste Management and Contaminated Site Treatment, Technische Universität Dresden, Pratzschwitzer Str. 15, D-01796 Pirna, Germany
- Heide, P., Institute of Waste Management and Contaminated Site Treatment, Technische Universität Dresden, Pratzschwitzer Str. 15, D-01796 Pirna, Germany
- Werner, P., Institute of Waste Management and Contaminated Site Treatment, Technische Universität Dresden, Pratzschwitzer Str. 15, D-01796 Pirna, Germany
- Schmidt, A.W., Department of Chemistry, Technische Universität Dresden, Bergstr. 66, D-01069 Dresden, Germany
- Theumer, G., Department of Chemistry, Technische Universität Dresden, Bergstr. 66, D-01069 Dresden, Germany
- Knölker, H.-J., Department of Chemistry, Technische Universität Dresden, Bergstr. 66, D-01069 Dresden, Germany

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