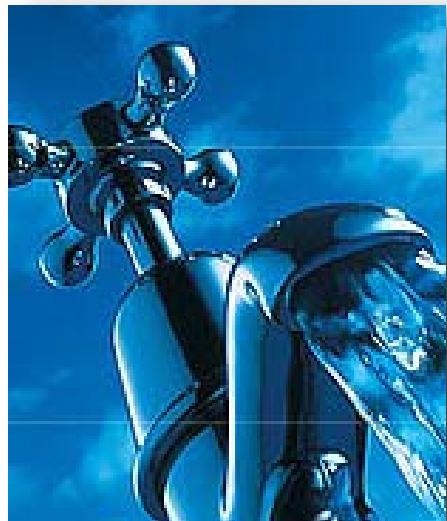


International Symposium for HPTLC
6th to 8th July 2011, Basel

Application of TLC-MS in water analysis



**Stefan C. Weiss^{1,2}, Wolfram Seitz¹,
Wolfgang Schulz¹ and Walter H. Weber¹**

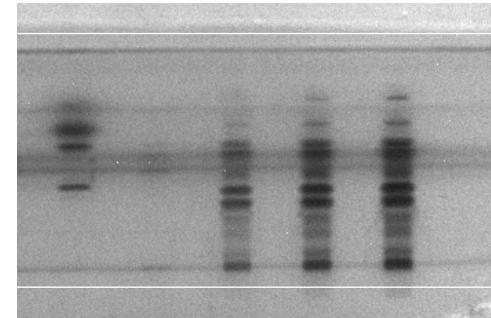
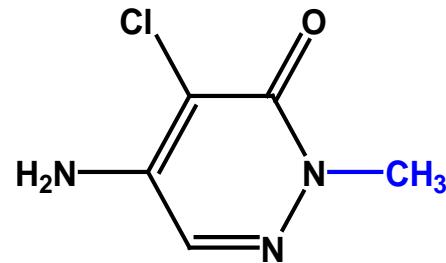
¹ Zweckverband Landeswasserversorgung
Laboratory for Operation Control and Research
Langenau, Germany

² Leuphana Universität Lüneburg
Institute for Environmental Chemistry, Germany

E-Mail: seitz.w@lw-online.de

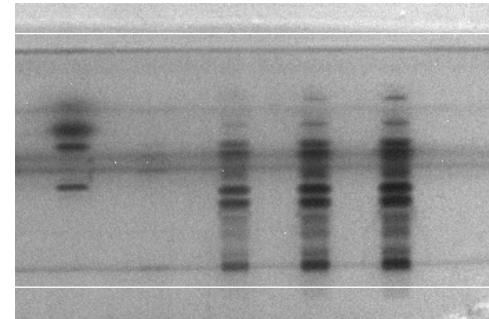
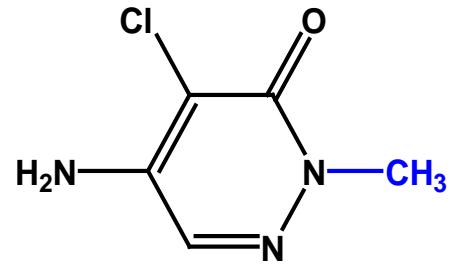
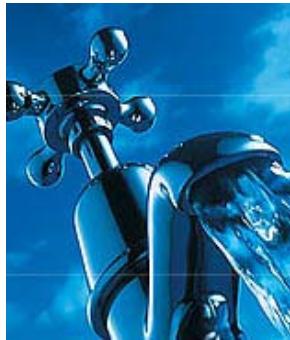
Structure

- Introduction
- Ground water contamination from synthetic turf
- Ozonation reaction products
- Conclusion

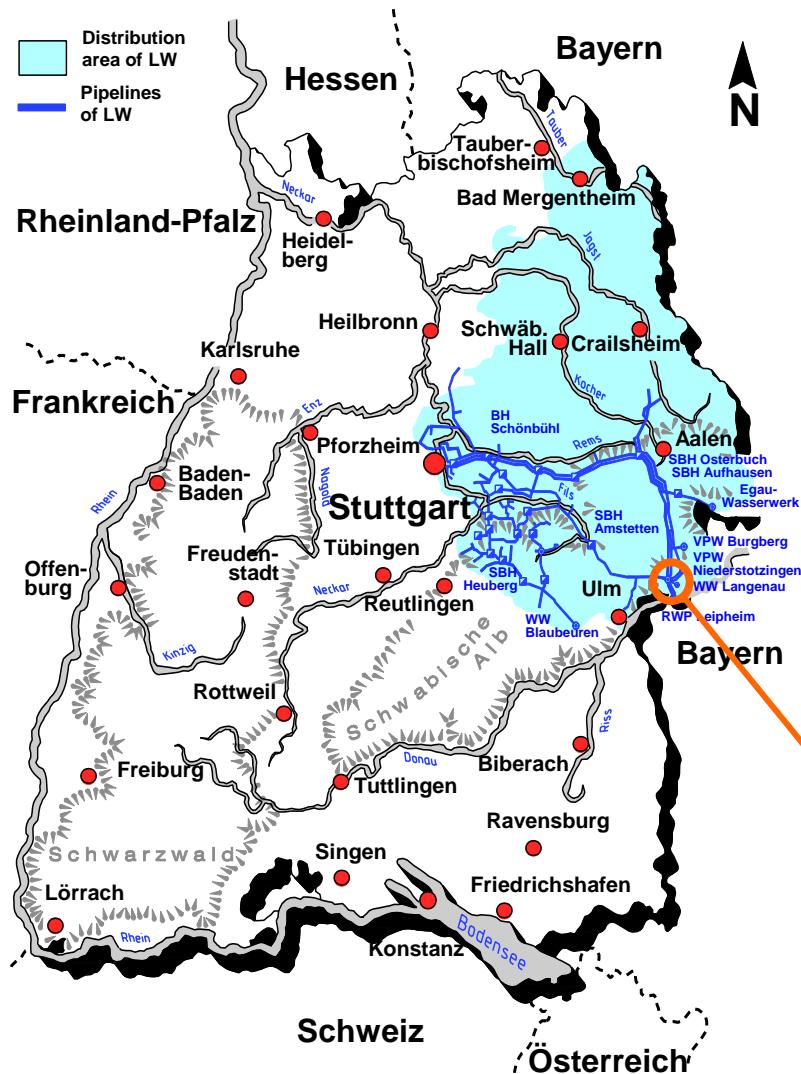


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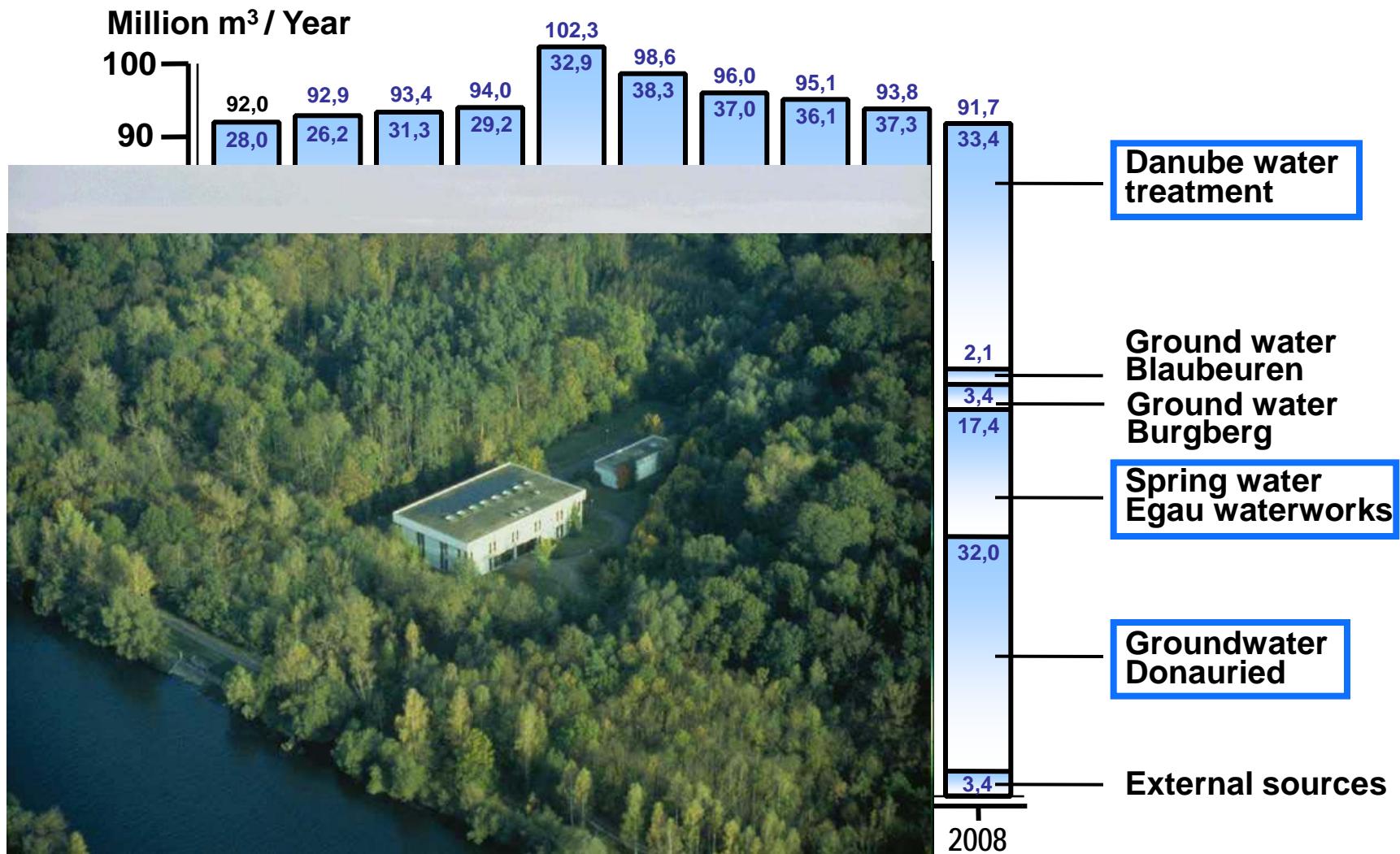


Distribution area of LW in South West Germany

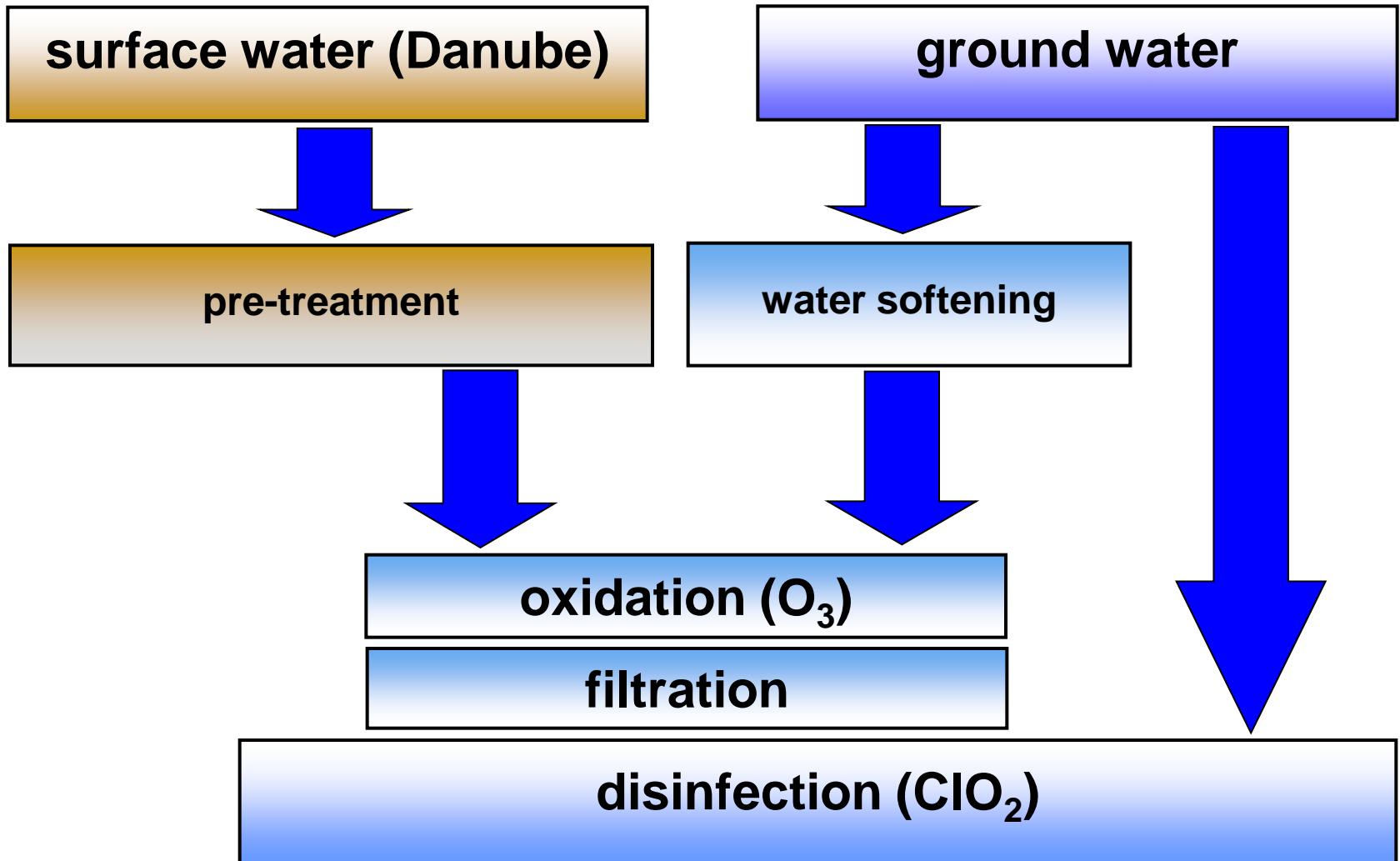


- Distribution area in South West Germany
 - 3 Million customers within distribution area
 - Long-distance water fraction approx. 50%
- Langenau Waterworks**

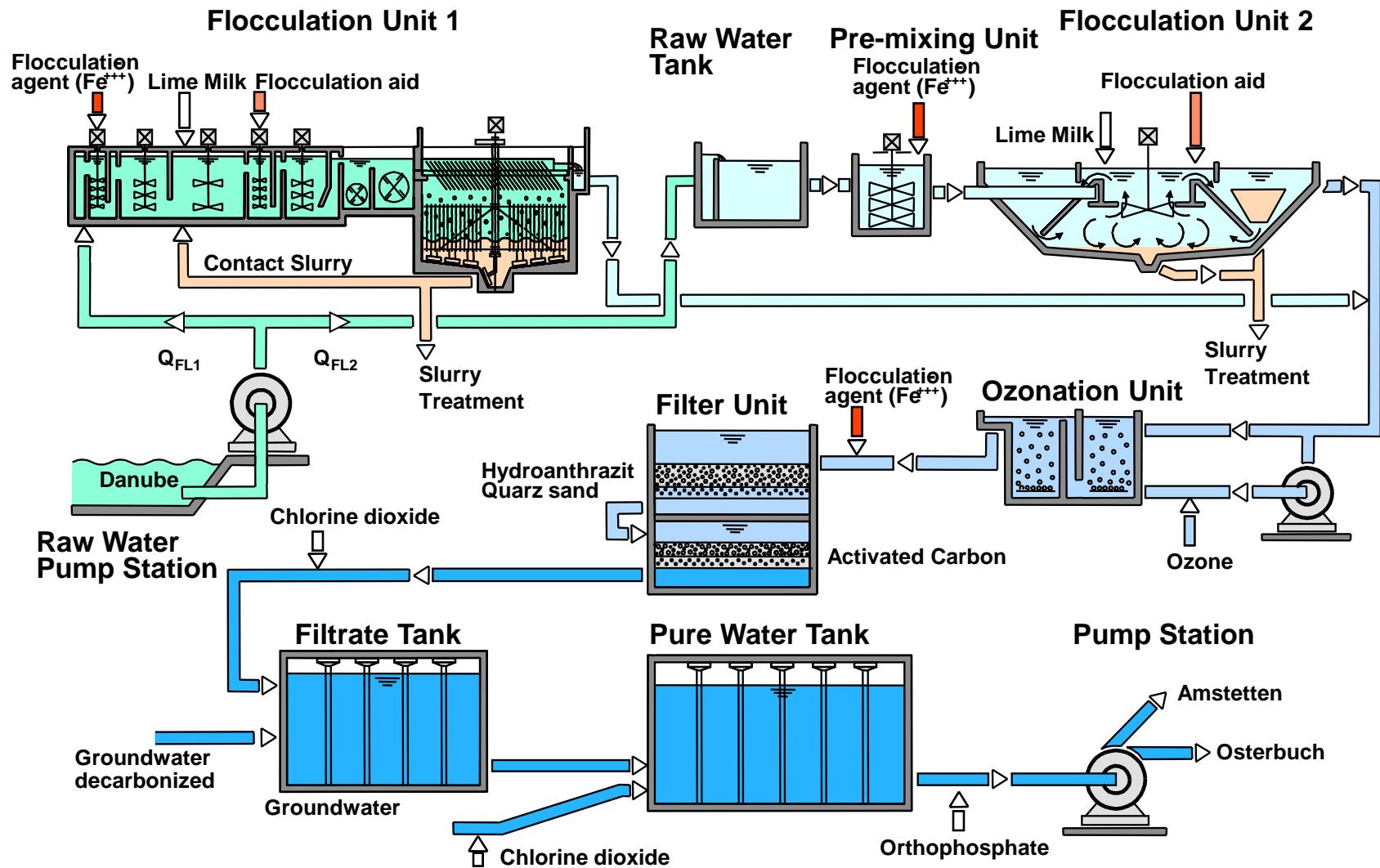
Water treatment from different resources



Water treatment at Langenau waterworks

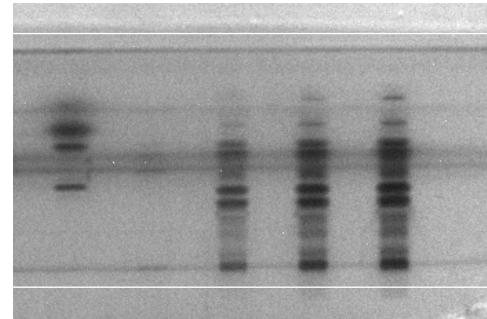
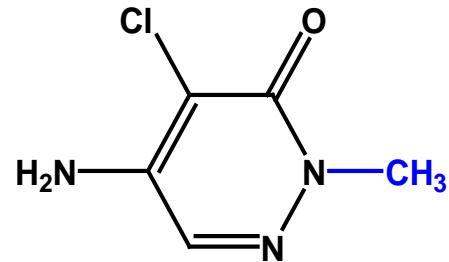


Treatment of Danube water at Langenau waterworks

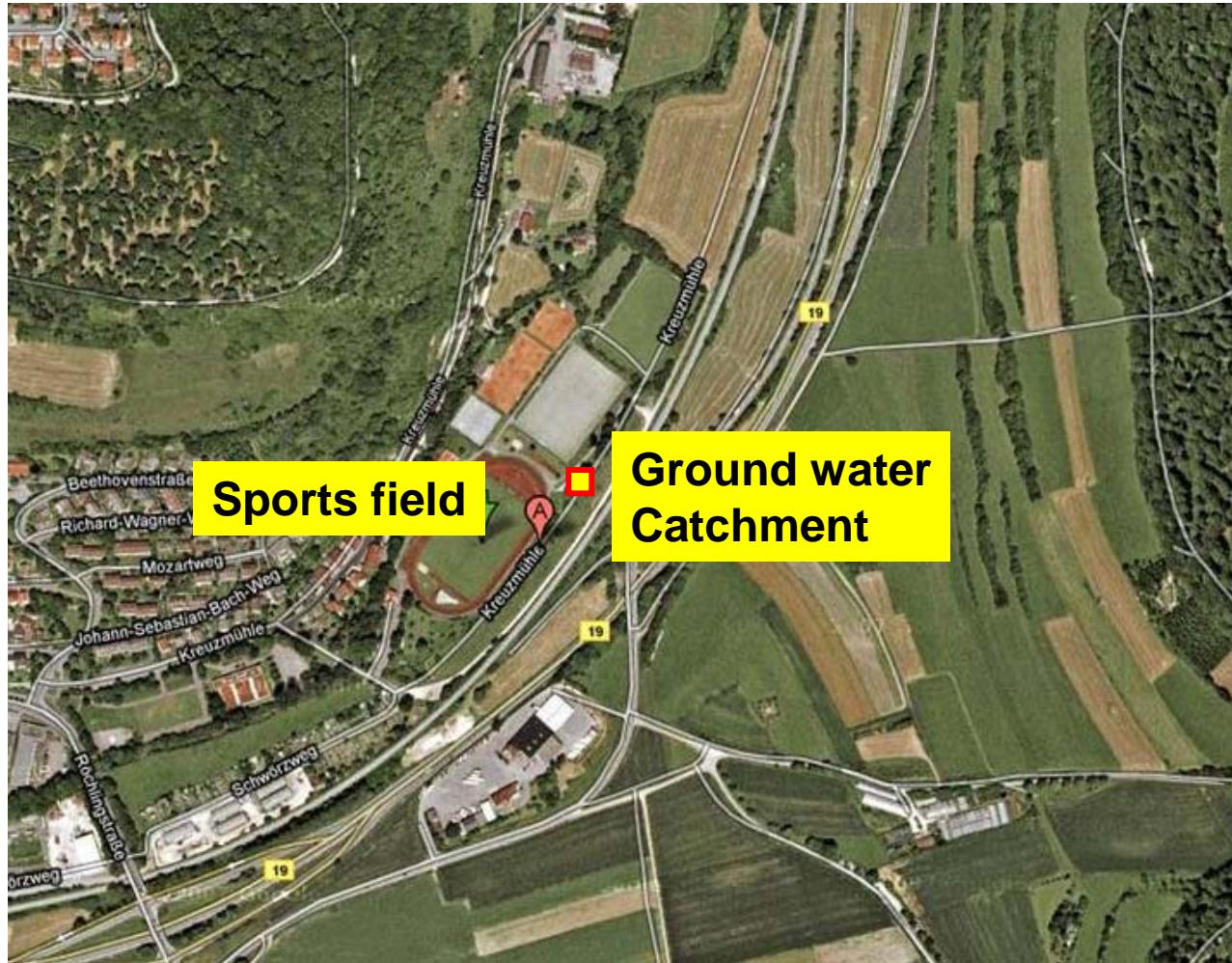


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Aerial photo of the region of interest



Ref.: Google Maps

Simulation of leaching synthetic turf with water

Synthetic turf:

PUR rubber granulate (elastic layer)



Leaching test:

(analog DIN 38414-S4)

Elution of 40 g sample with 80 g water

Duration: 24 h

Liquid/liquid extraction of the eluate

Extraction solvent: Methyl tert-butyl ether

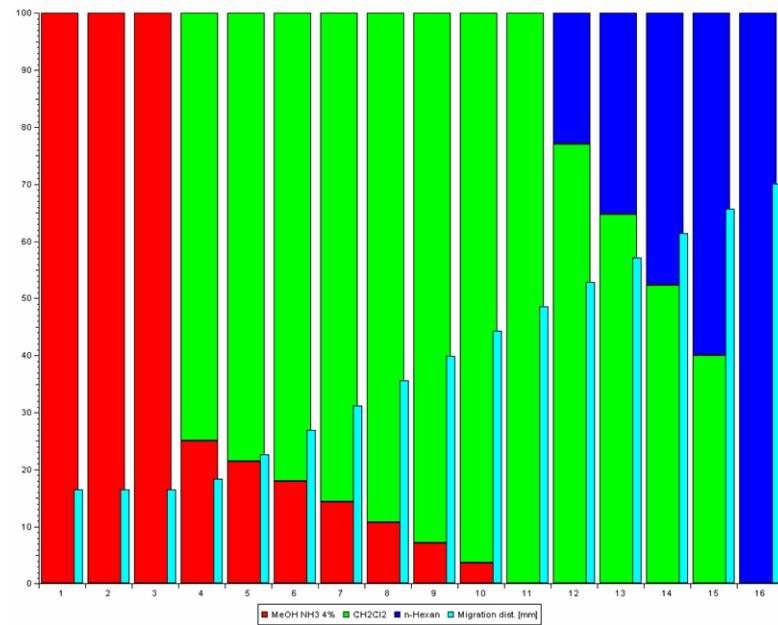
Blank: Ultra pure water



HPTLC/AMD analysis

Chromatography:

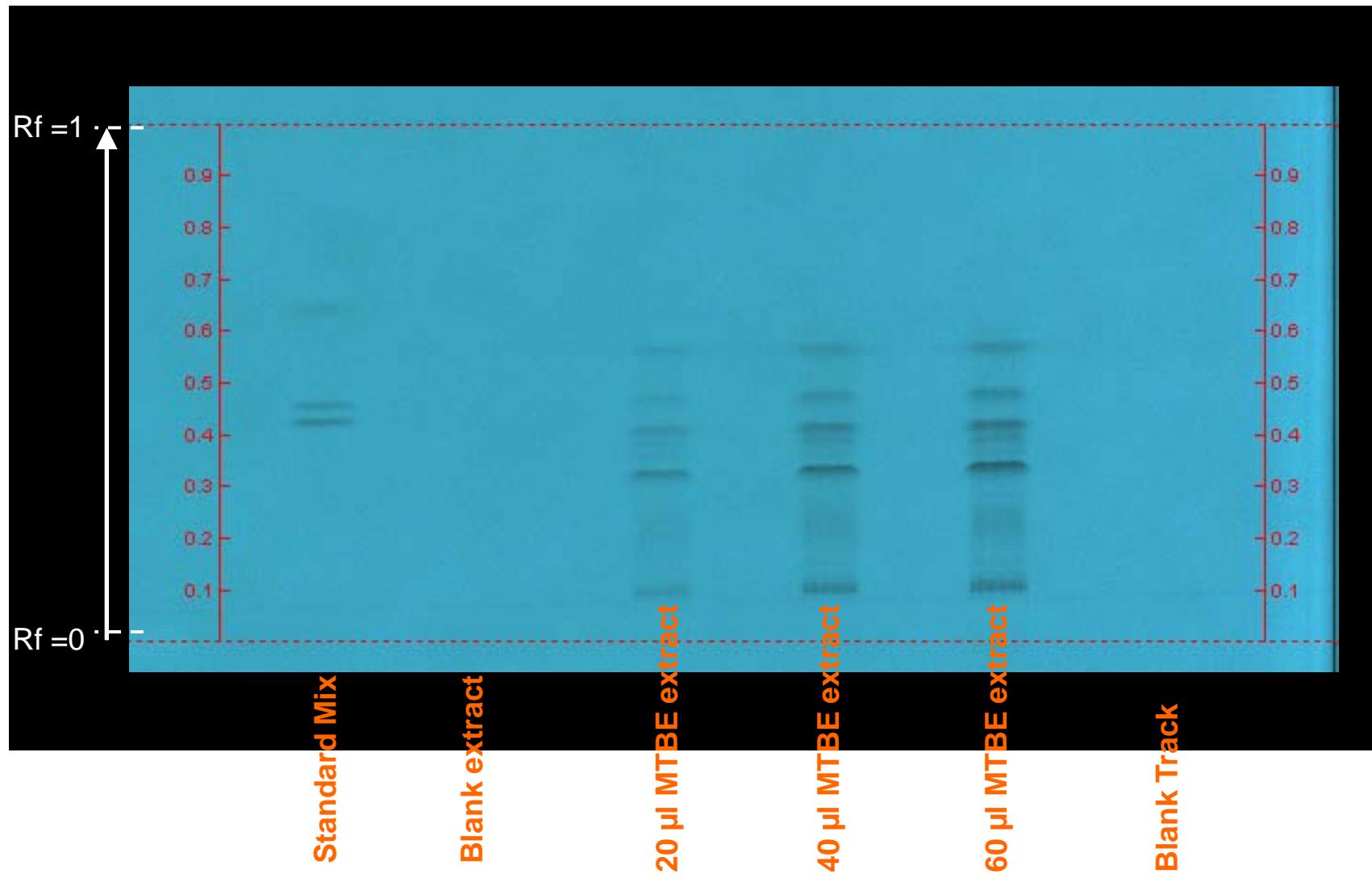
Eluents: MeOH:NH₃ (4%)
Dichloromethane
n-Hexane



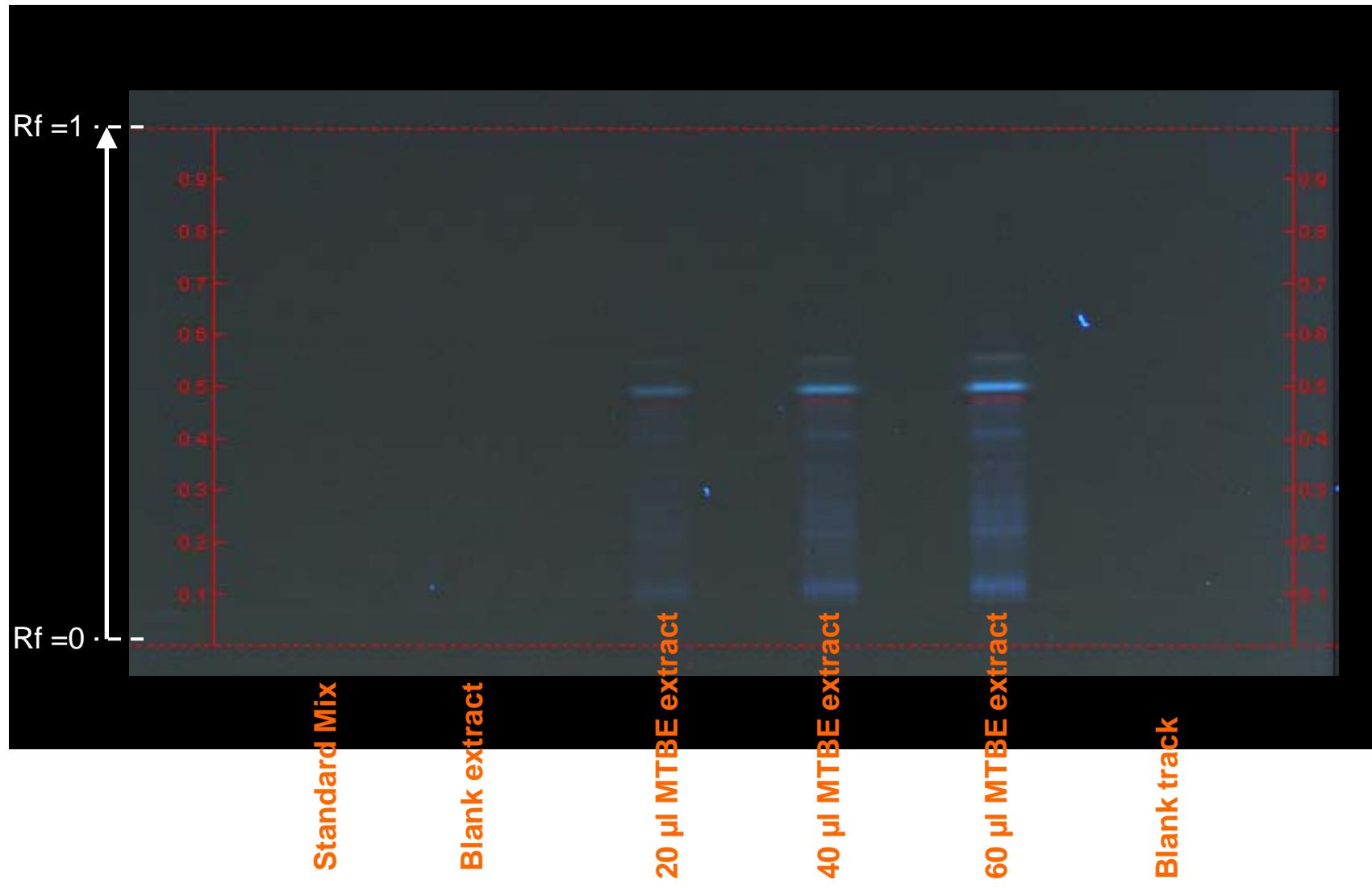
Detection:

- UV absorption (multiple wavelength scan)
- Fluorescence quenching at 254 nm
- Fluorescence, excitation at 366 nm
- Luminescence inhibition test

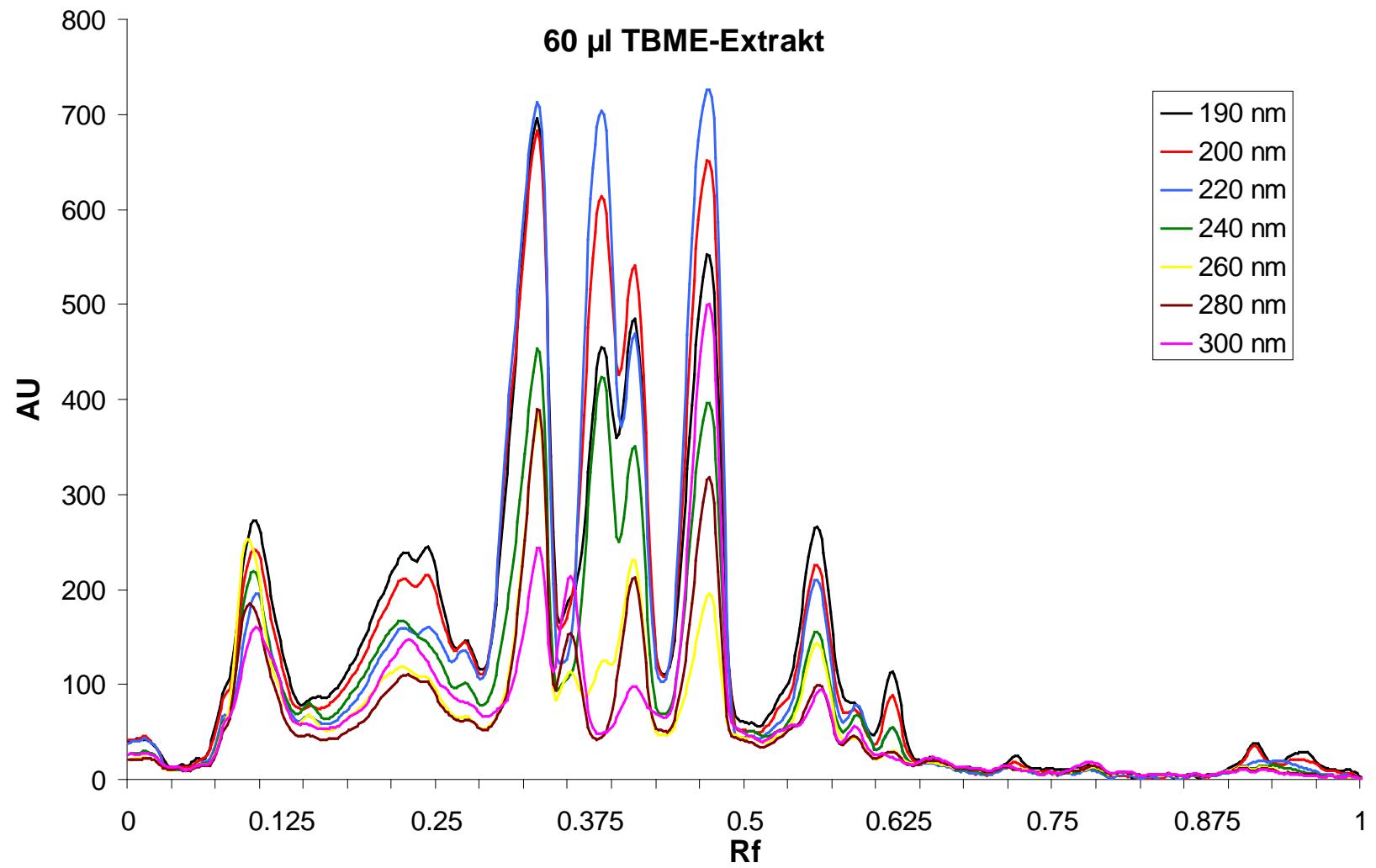
Fluorescence quenching at 254 nm



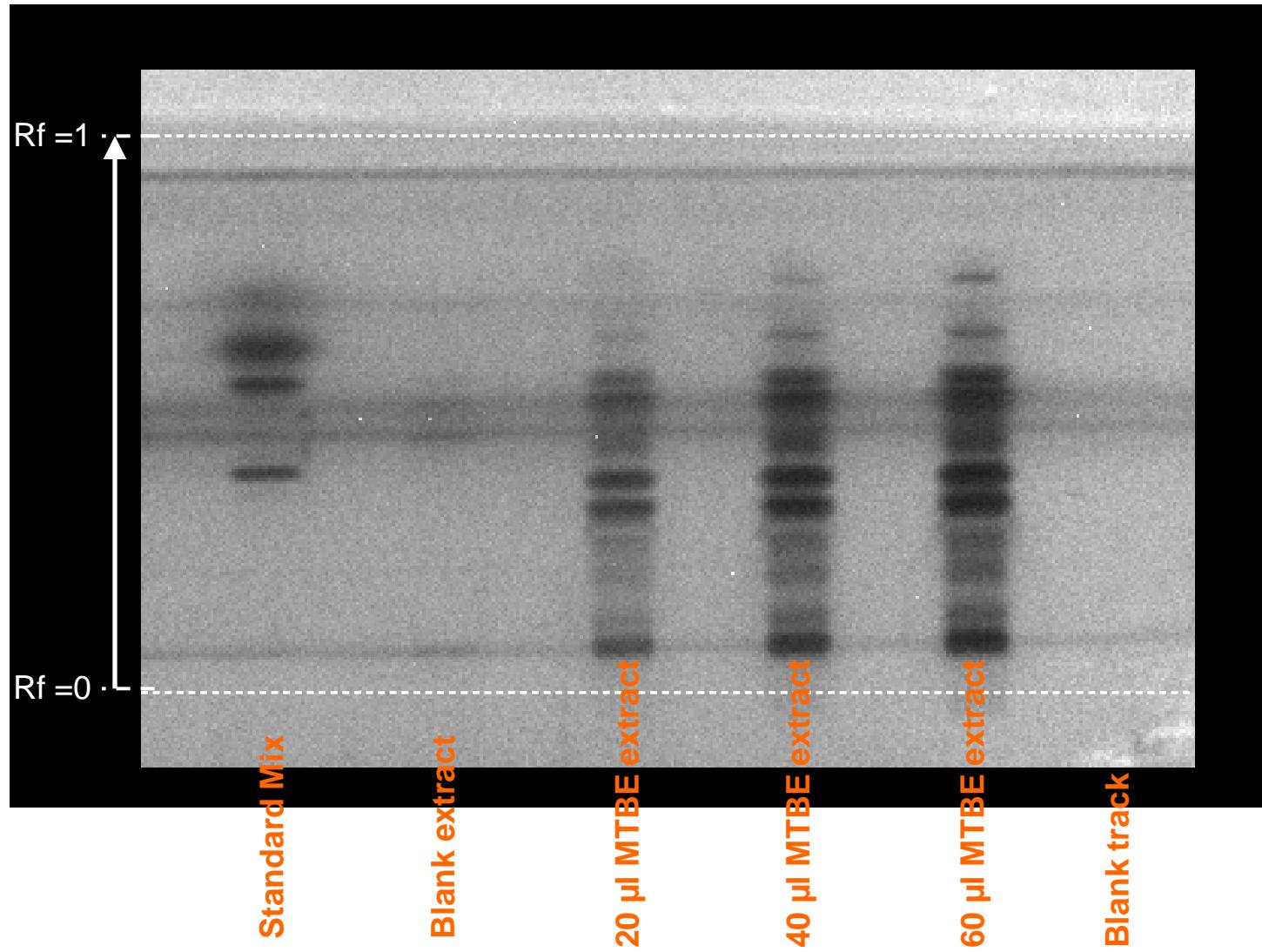
Fluorescence (excitation at 366 nm)



UV absorption (multiple wavelength scan)

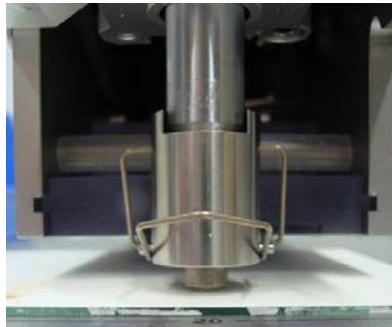
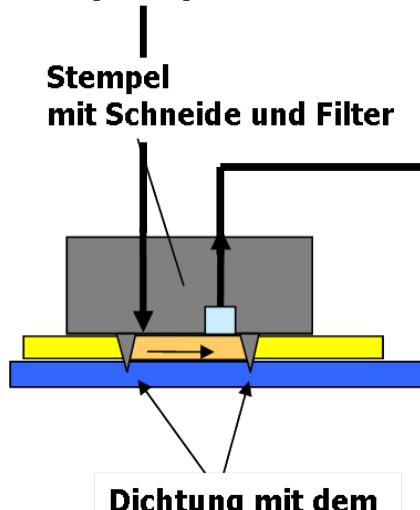


Detection of luminescence inhibition (*Vibrio fischeri*)

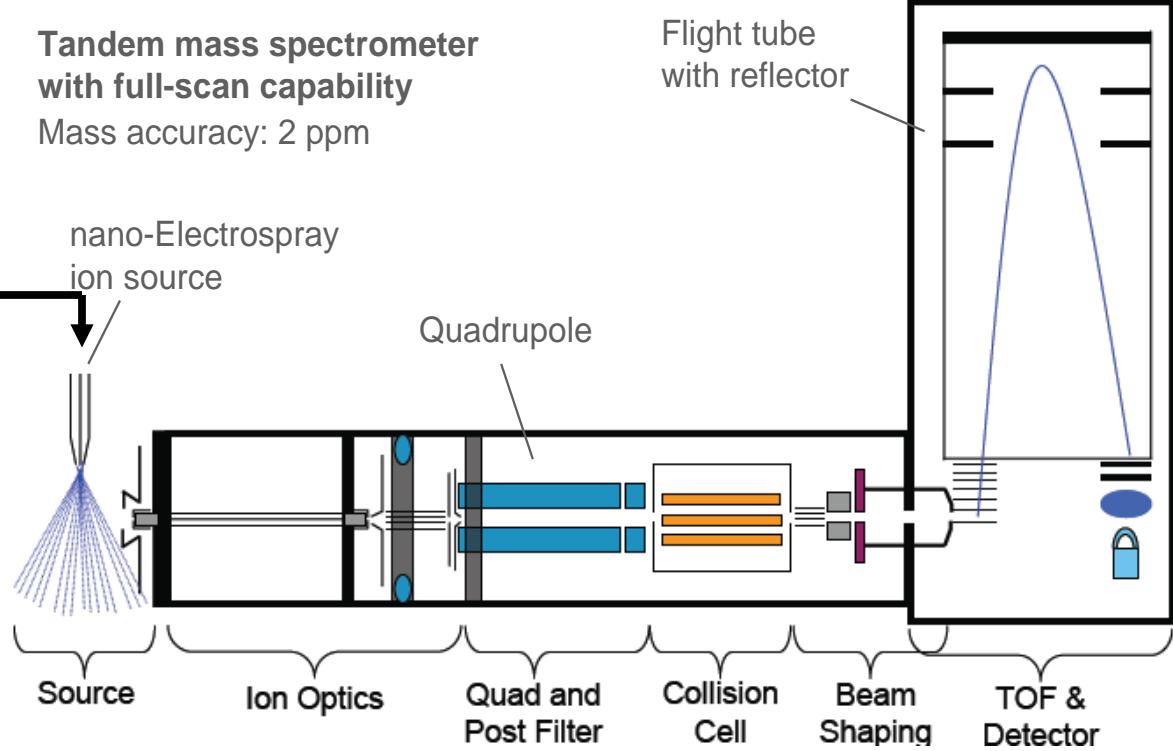


Transfer of substances via HPTLC-MS interface and MS analysis

Eluent from
HPLC pump

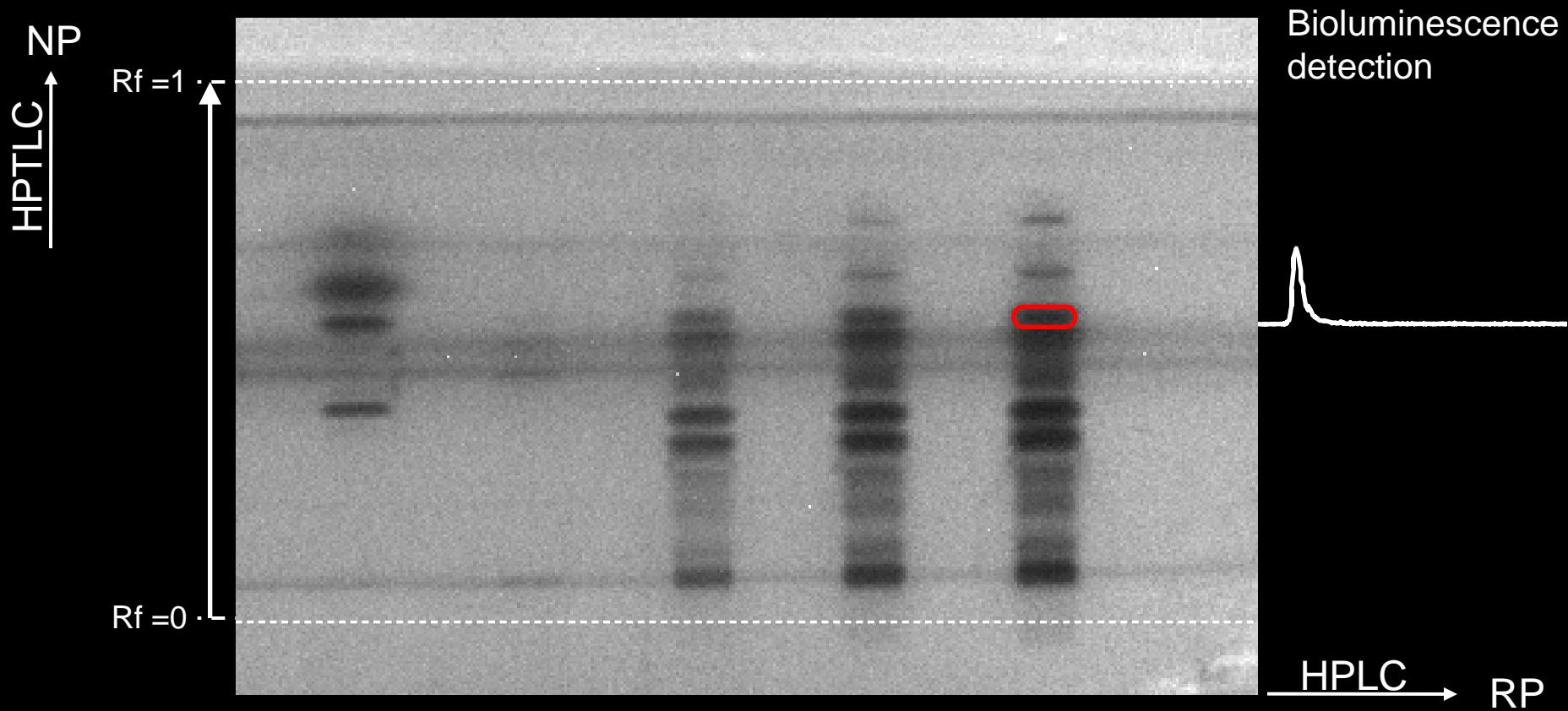


Tandem mass spectrometer
with full-scan capability
Mass accuracy: 2 ppm

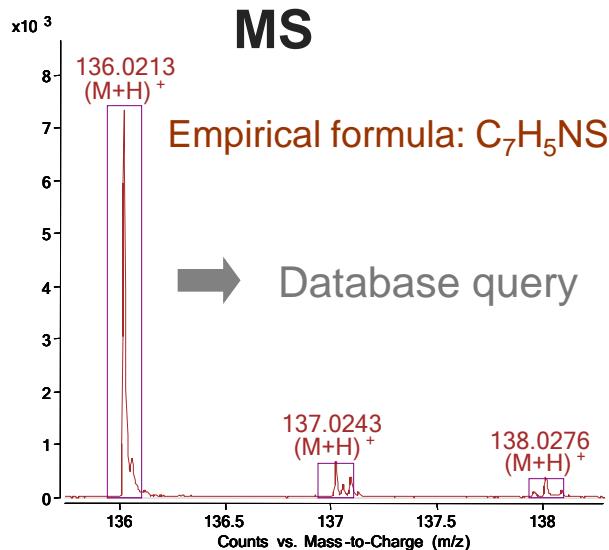


H. Luftmann (2004) Anal.
Bioanal Chem., 378, 964

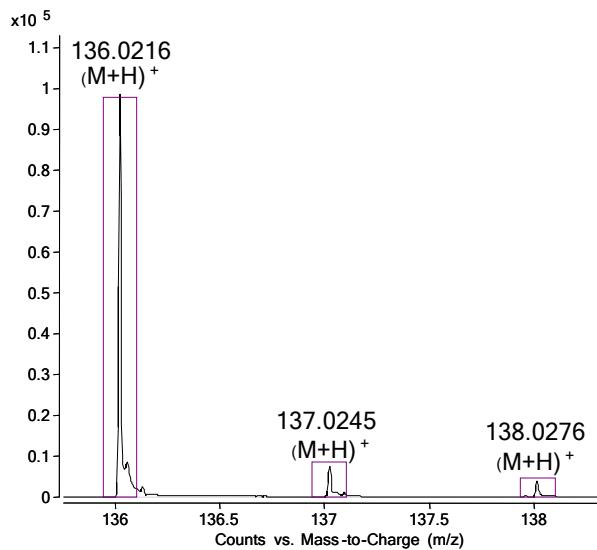
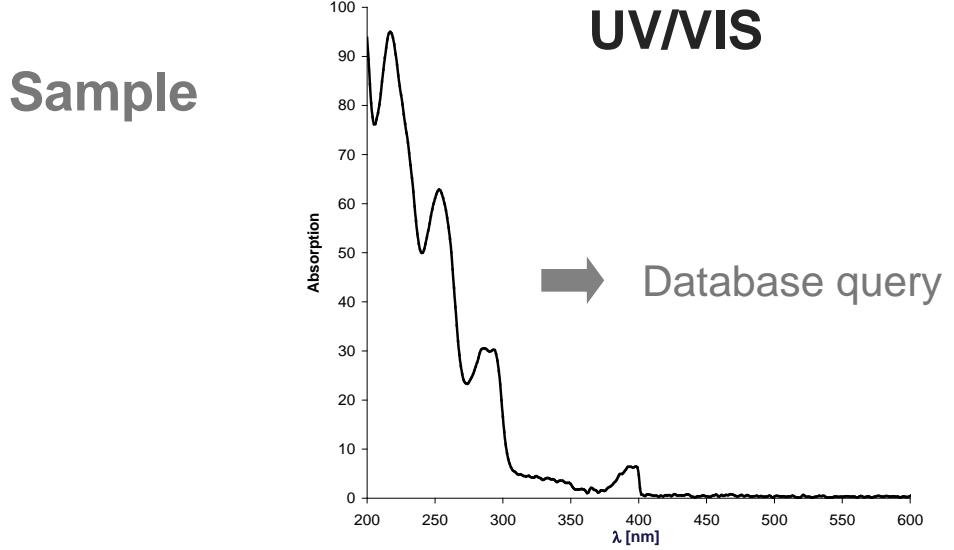
Detection of luminescence inhibition (*Vibrio fischeri*) and transfer of the substances via HPTLC-MS interface to MS



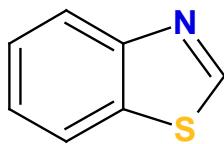
Identification of the unknown compound



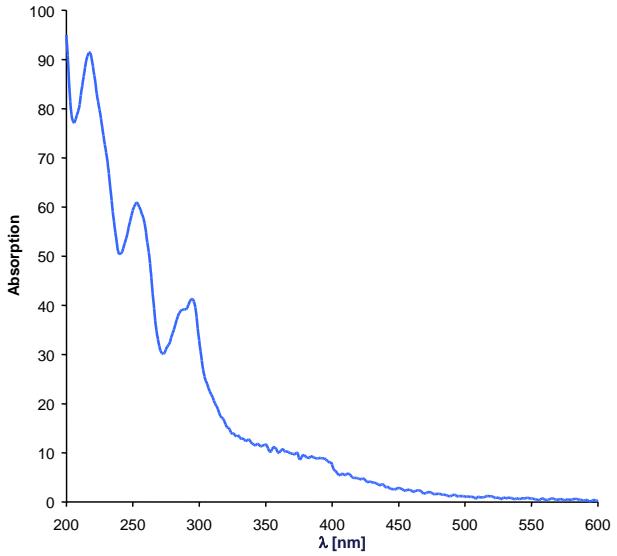
Sample



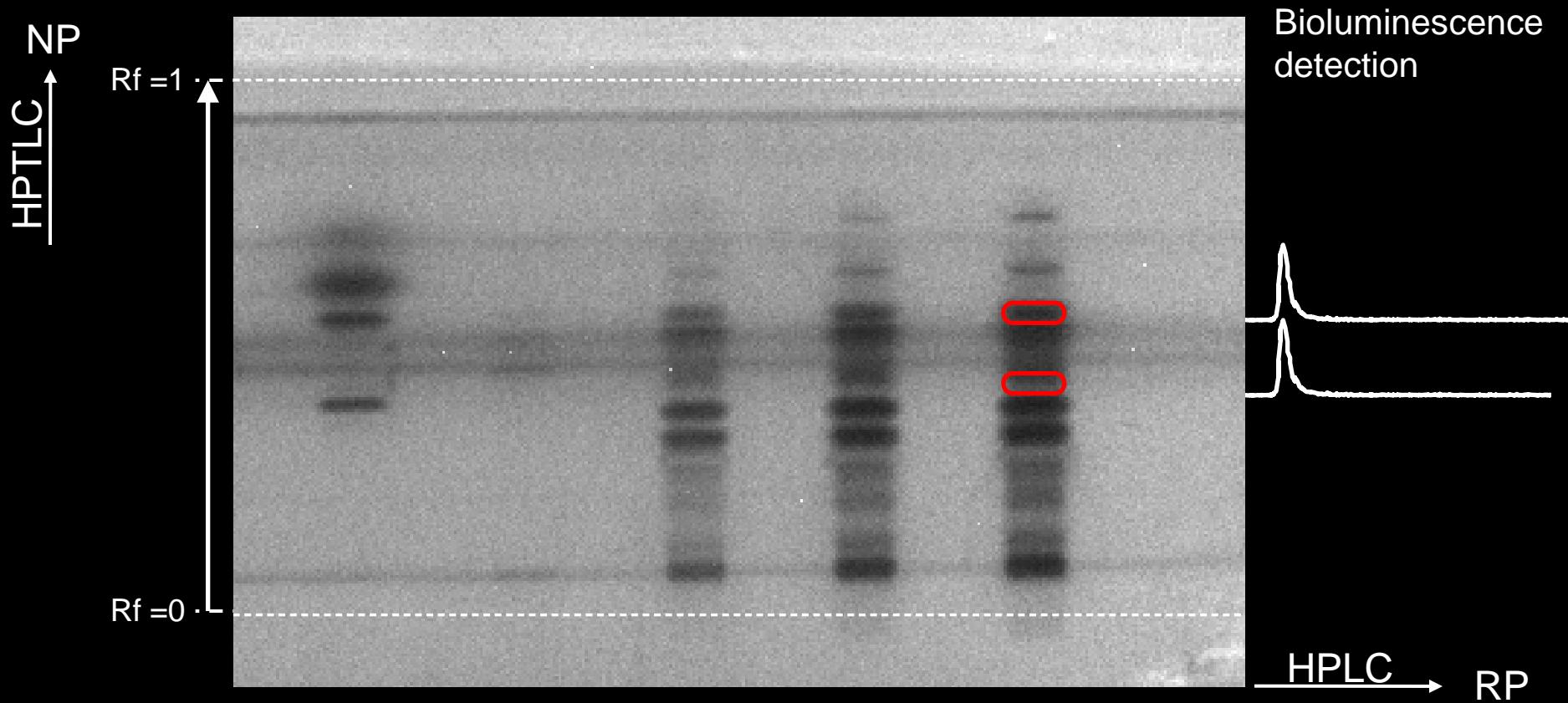
Reference



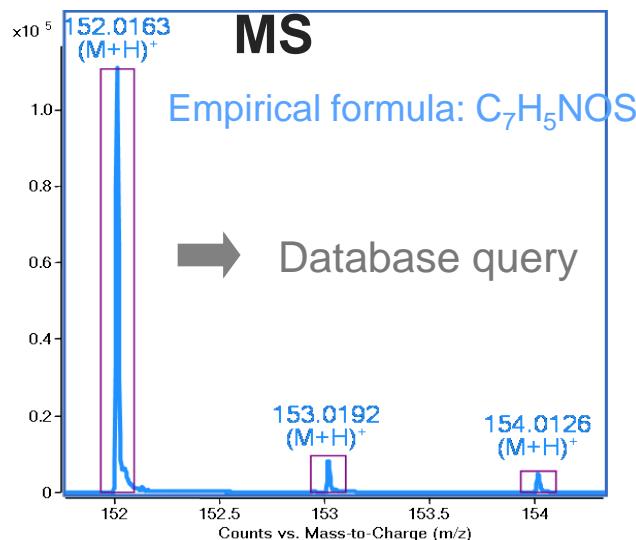
Benzothiazol



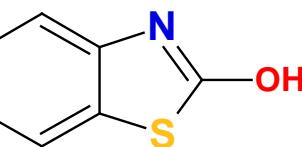
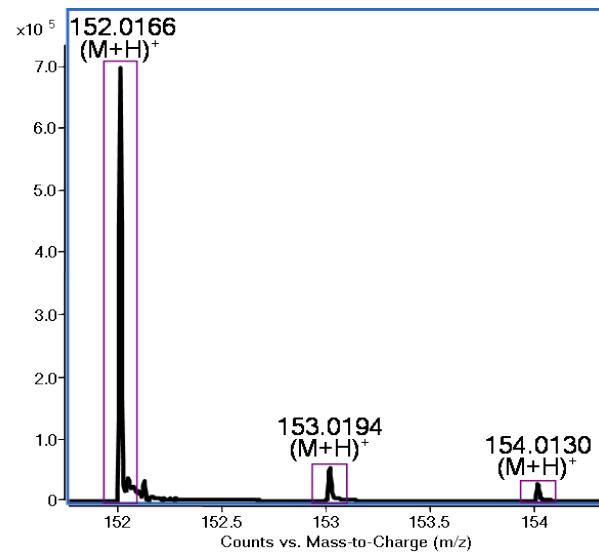
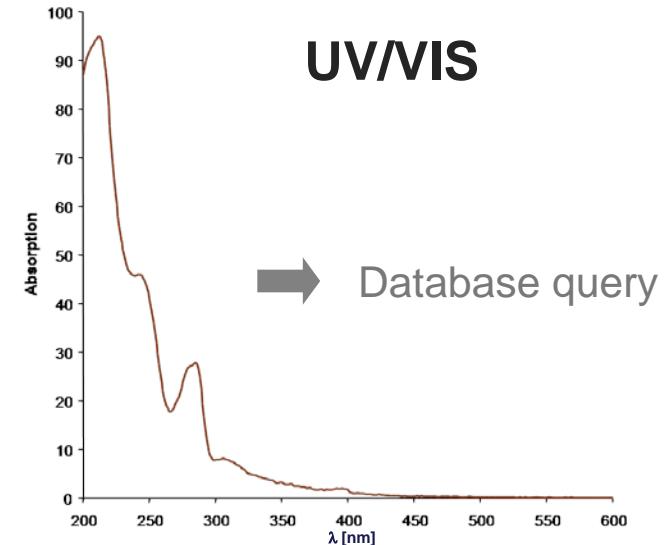
Detection of luminescence inhibition (*Vibrio fischeri*) and transfer of the substances via HPTLC-MS interface to MS



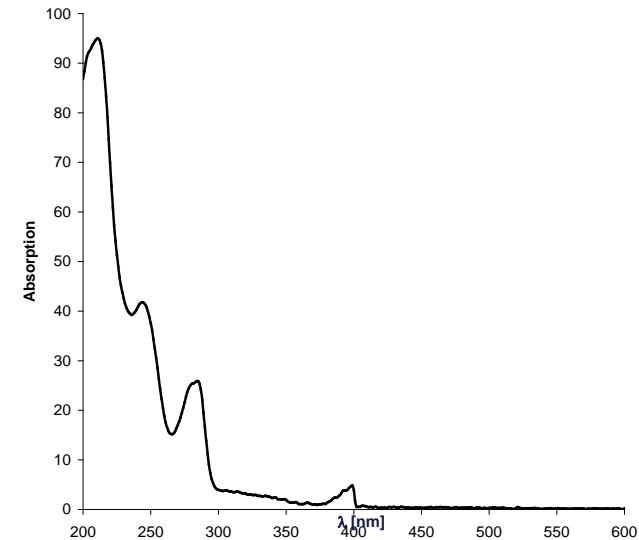
Identification of the unknown compound (II)



Sample

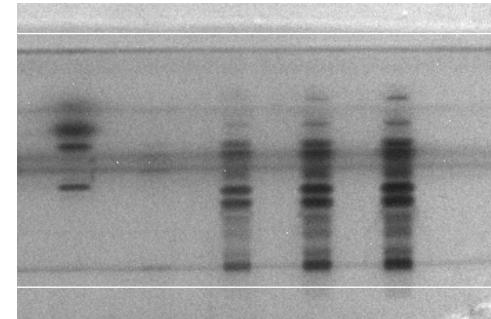
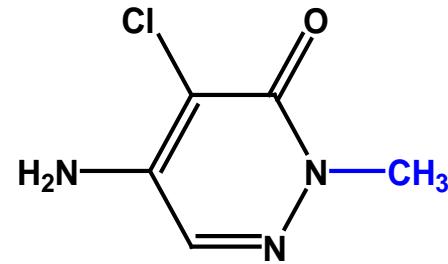


2-Hydroxybenzothiazol

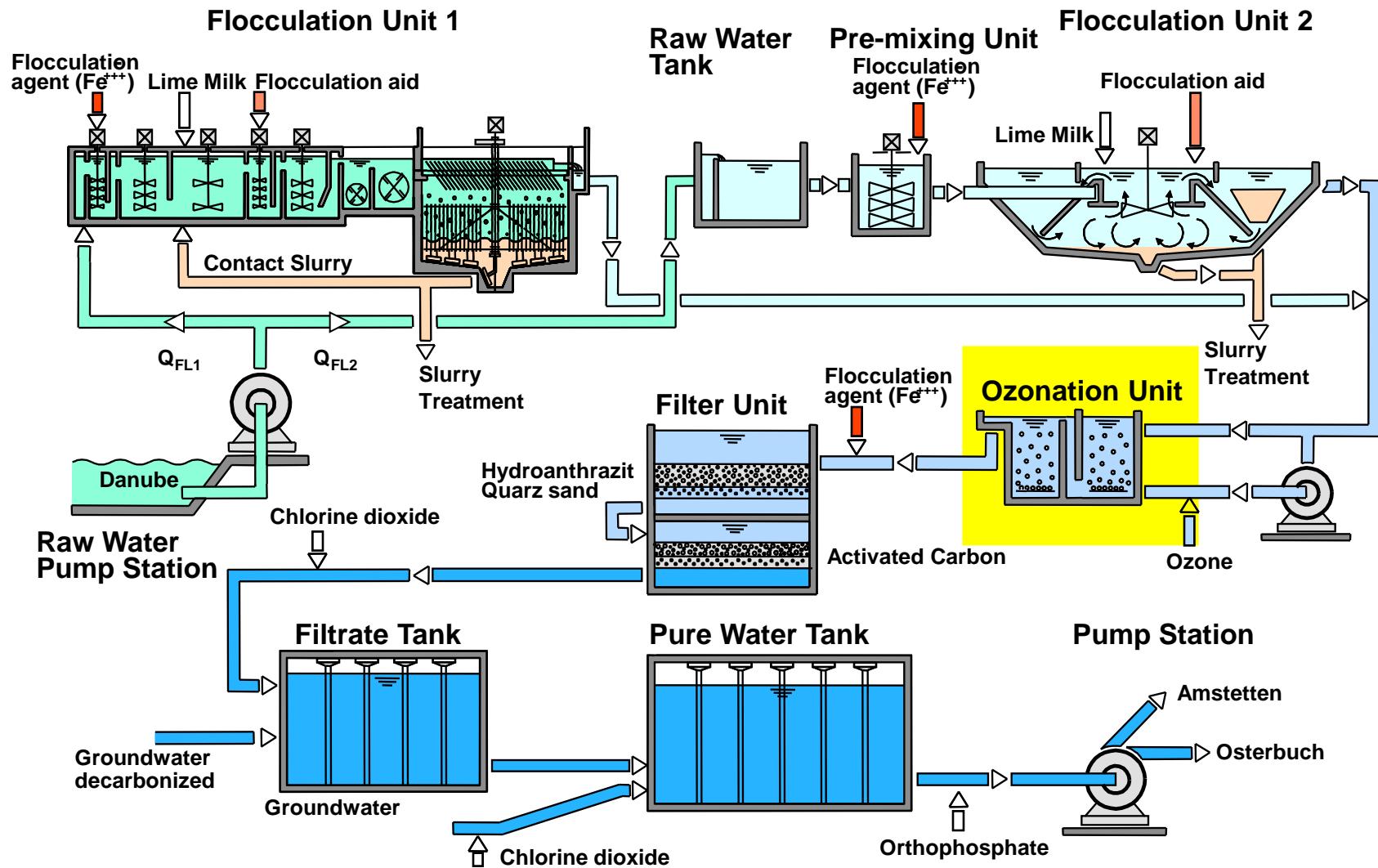


Structure

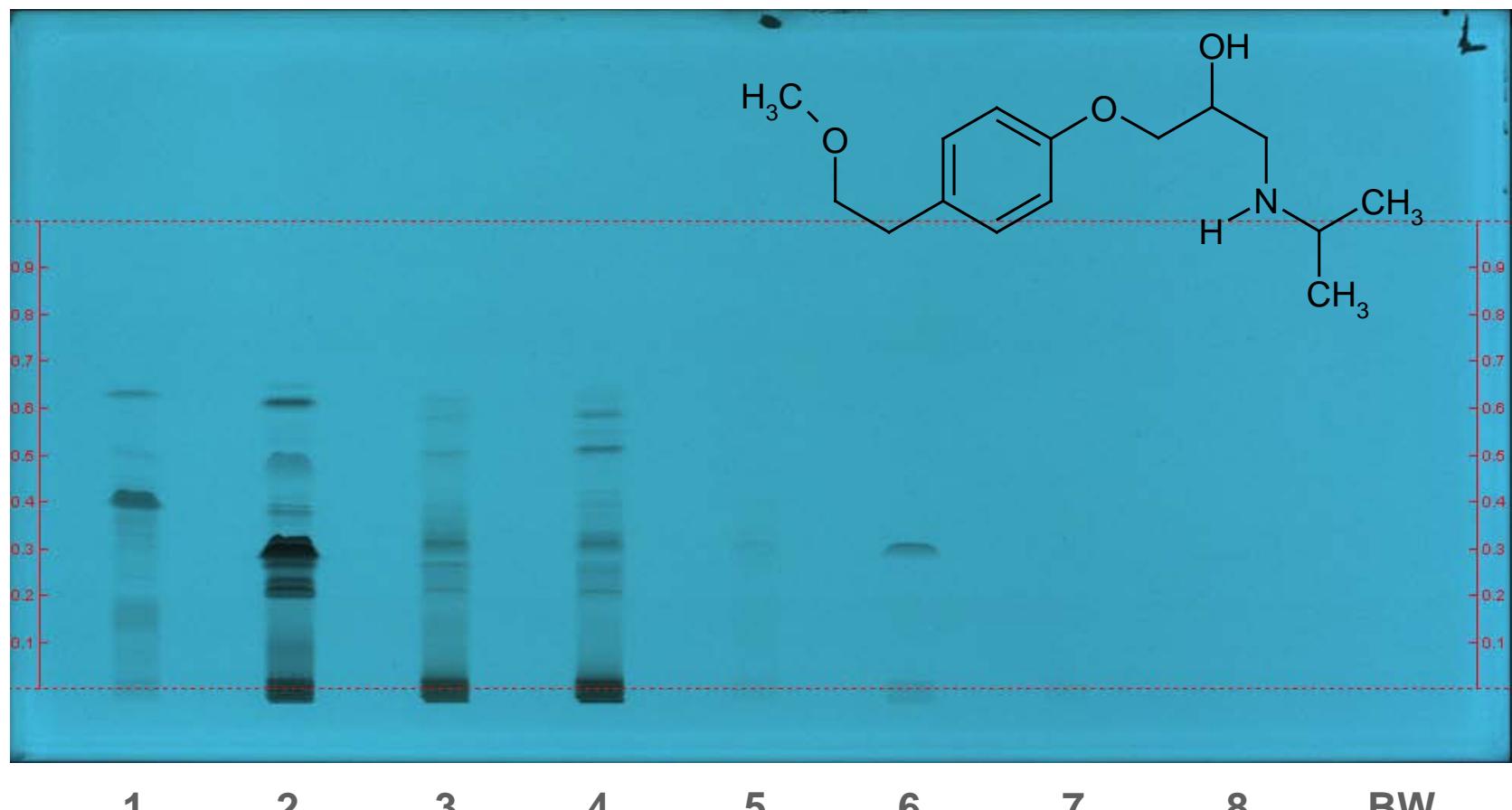
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Treatment of Danube water at Langenau waterworks

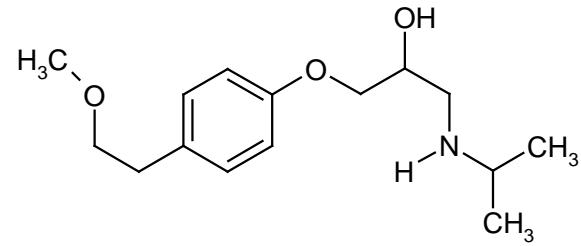
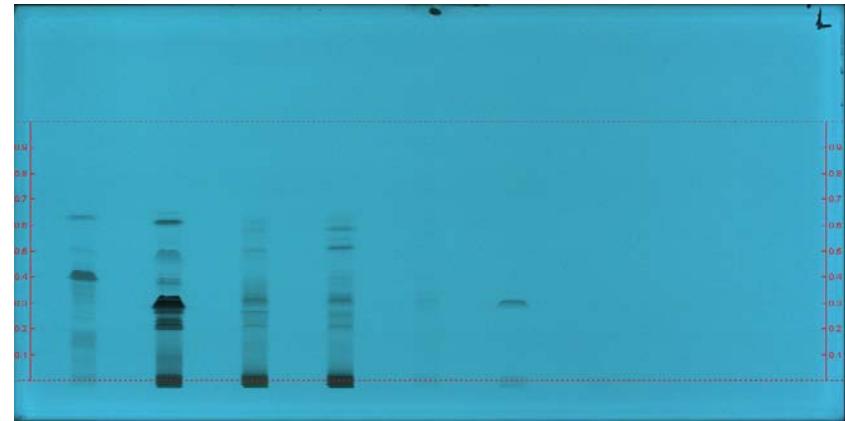
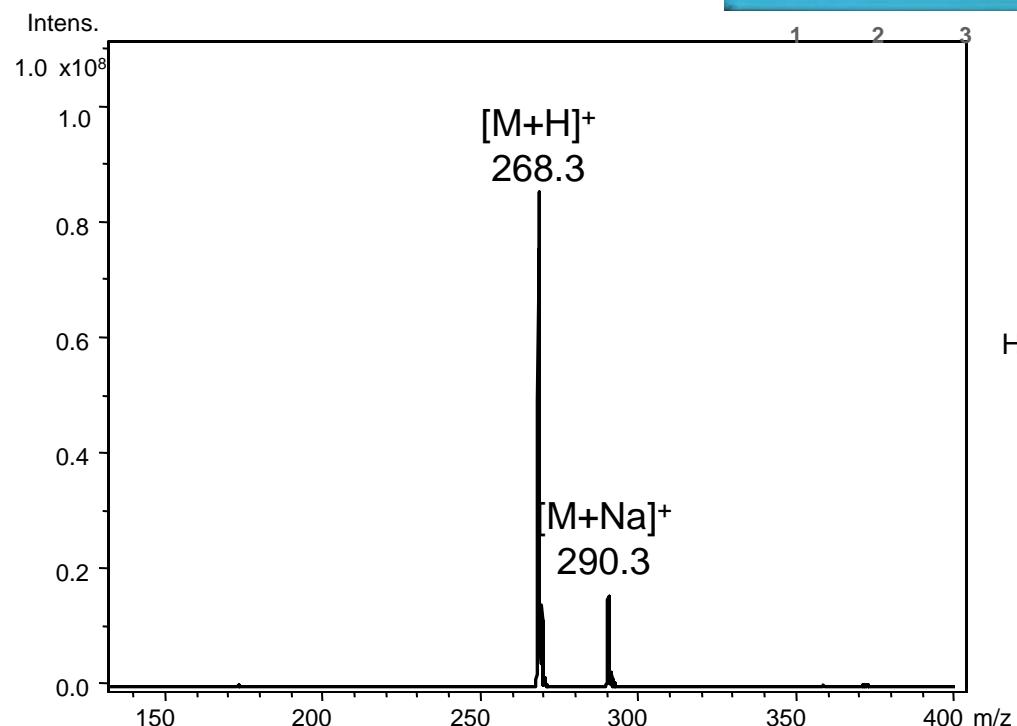


Oxidation of Metoprolol by ozone



Fluorescence quenching ($\lambda = 254$ nm)

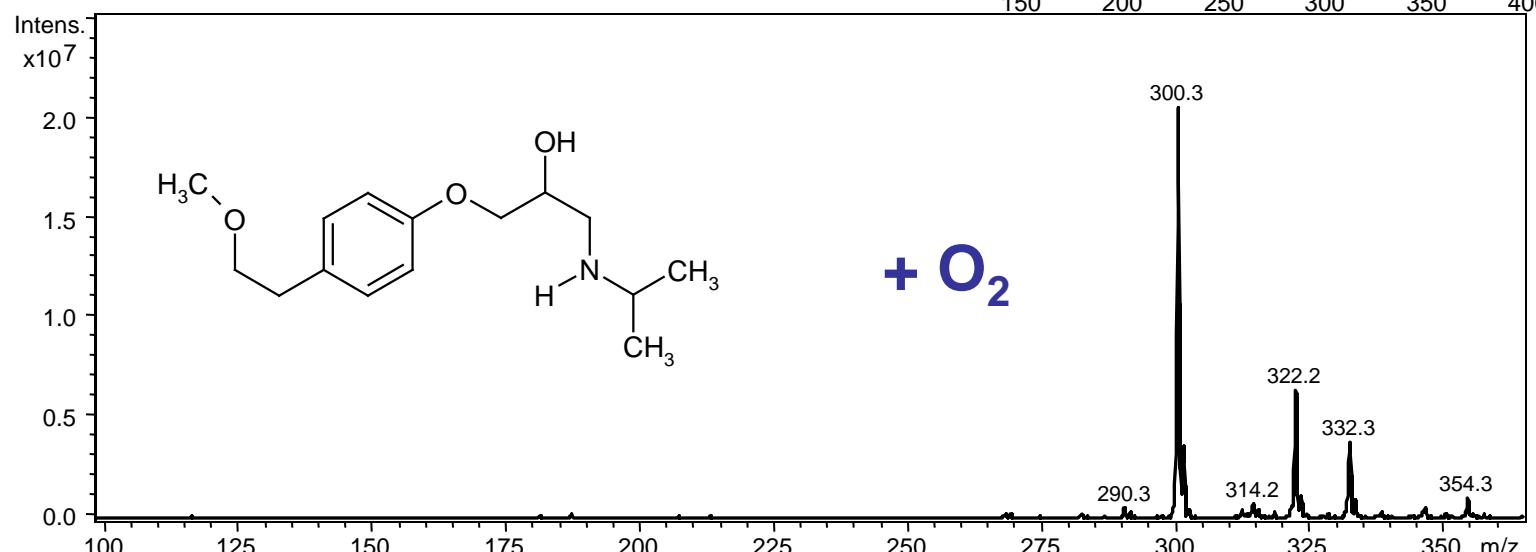
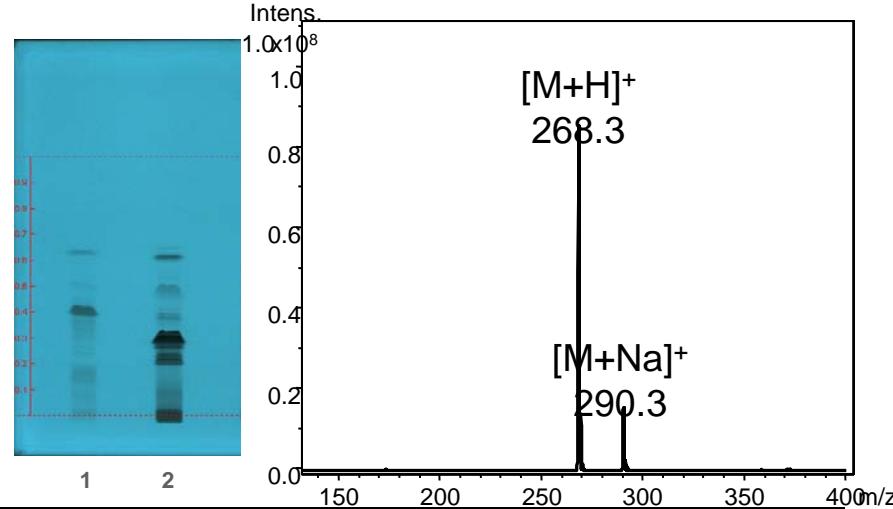
TLC-MS analysis of metoprolol



Metoprolol

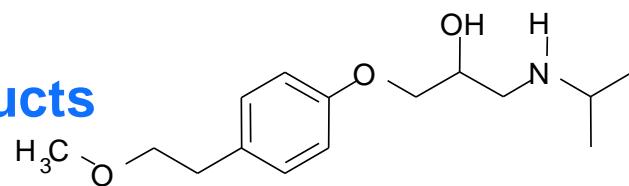
Track 6

TLC-MS analysis of oxidation by-products

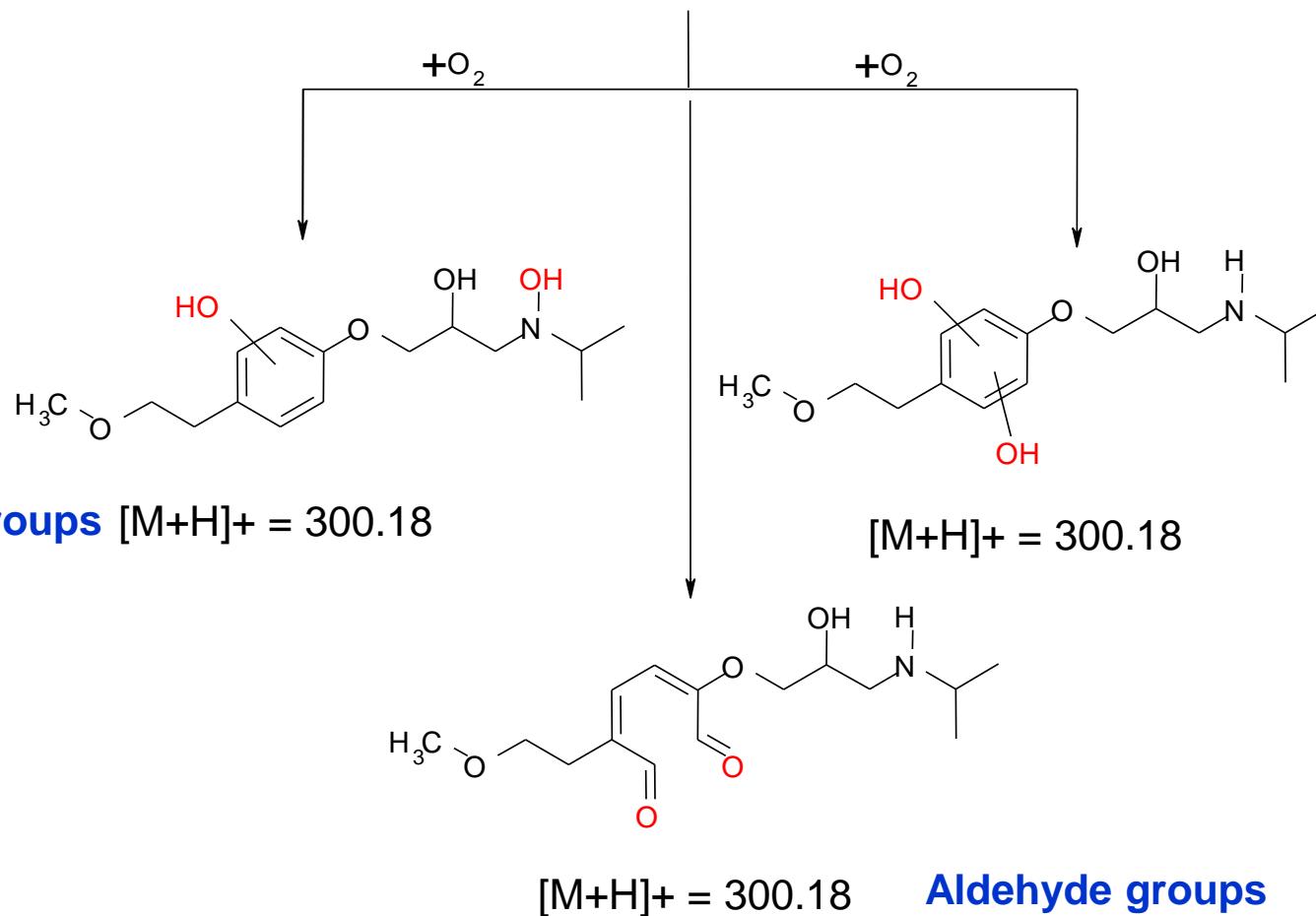


Track 2

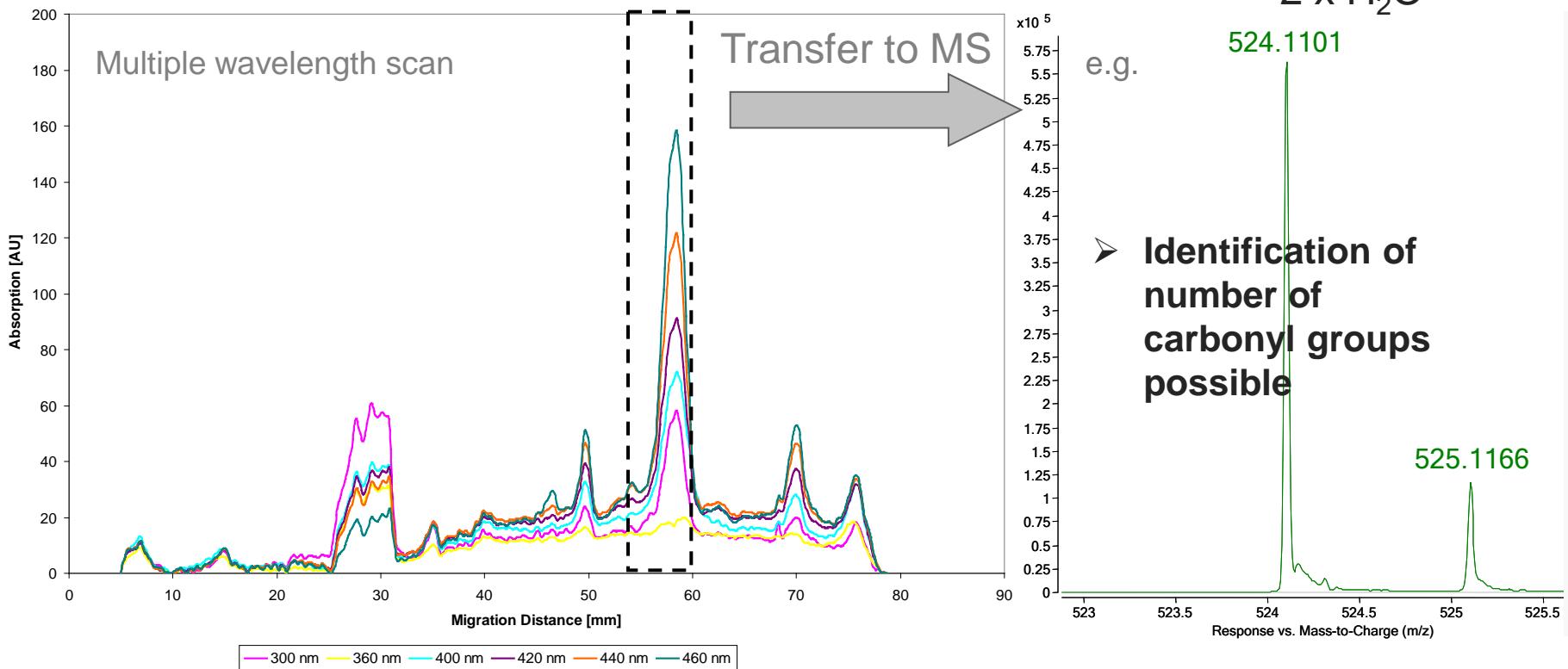
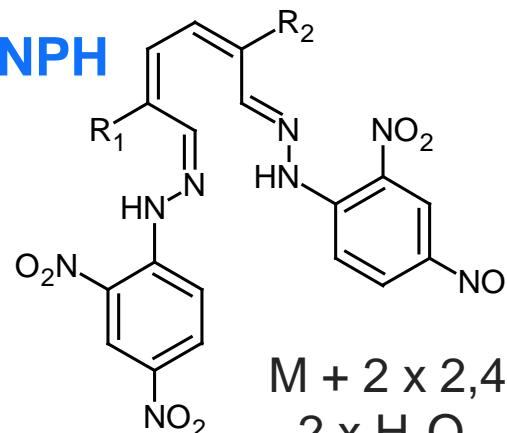
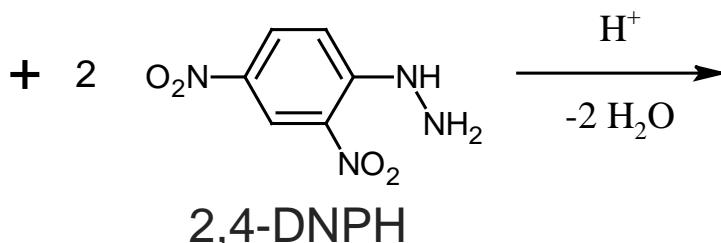
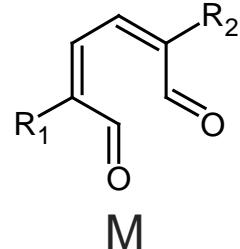
Metoprolol and oxidation by-products



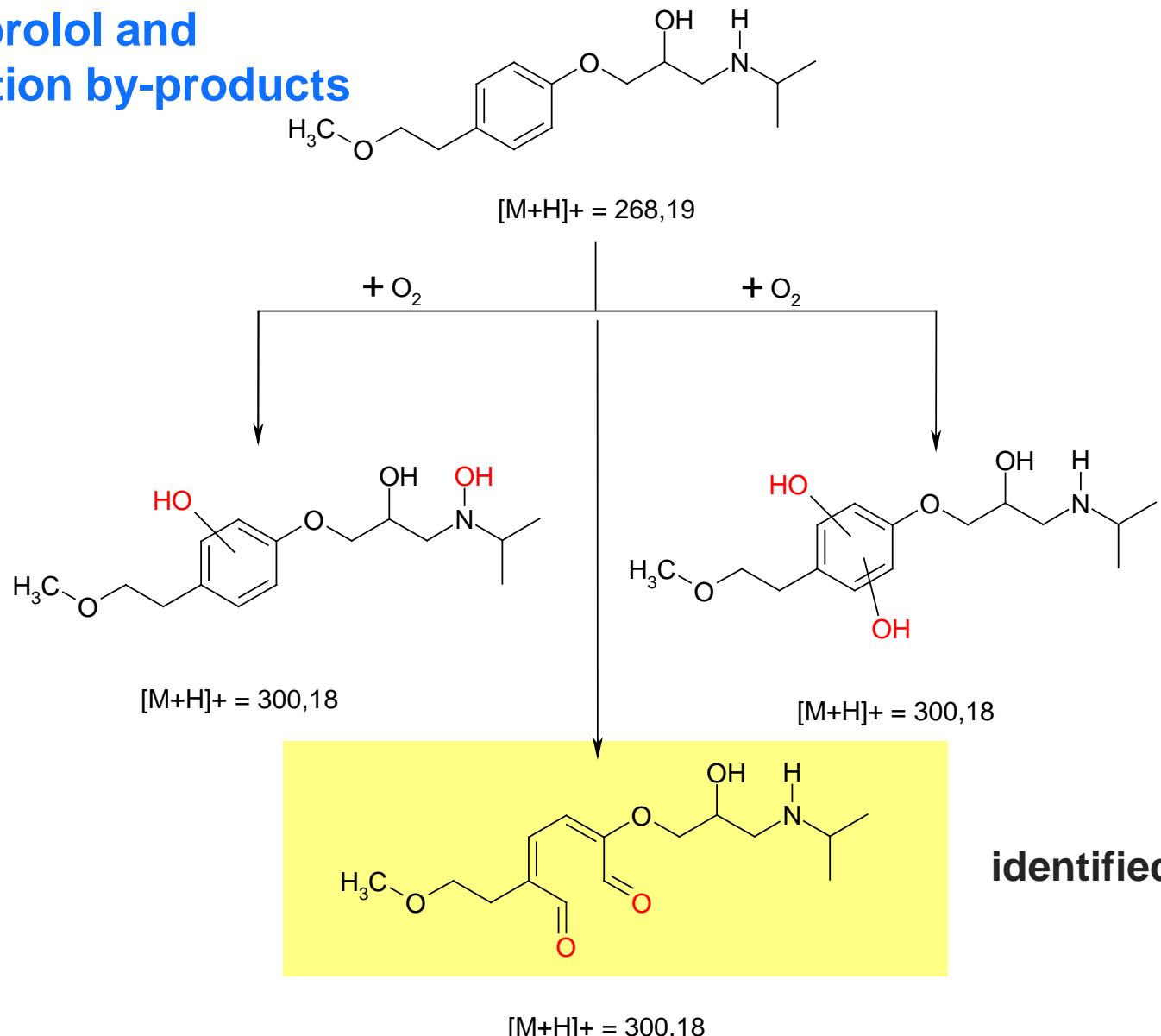
$[M+H]^+ = 268.19$



Detection of ketones and aldehydes using DNPH

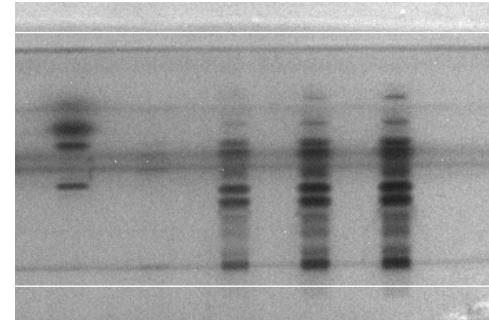
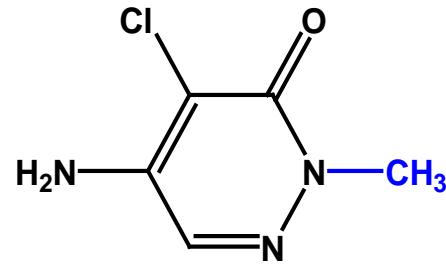
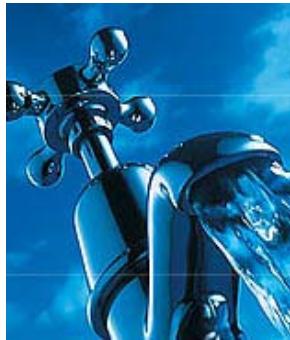


Metoprolol and oxidation by-products

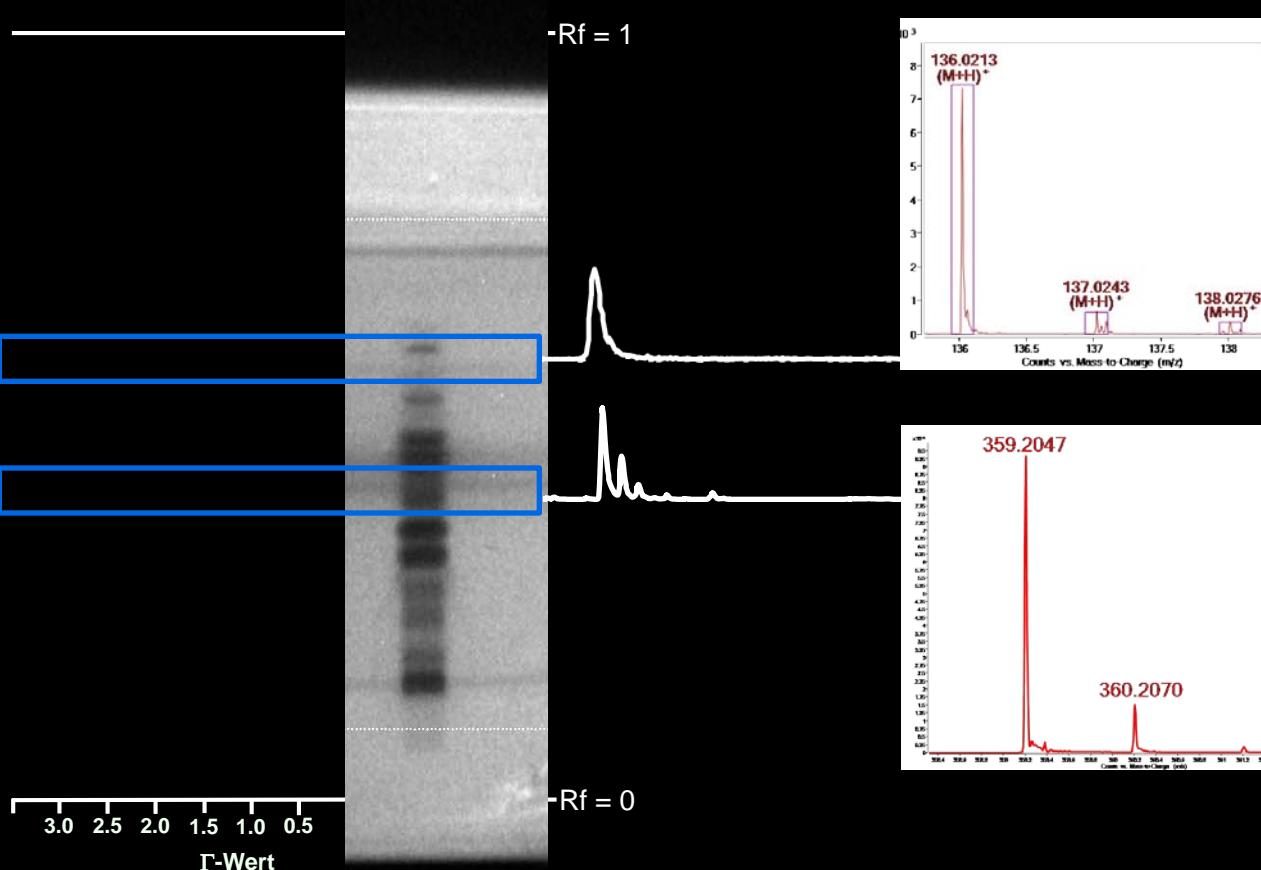


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Conclusion



Acknowledgments

Roger Albert
Alexander Müller
Walter H. Weber

and the member of staff at the
Laboratory for Operation Control and Research

Event note

8th Langenauer Wasserforum

**7th and 8th November 2011
Langenau, Germany**

**German Symposium and Exhibition
on Water and Environmental Analysis**

**“8 Years of development in organic trace analysis
with chromatography and mass spectrometry”**

Information: www.lw-online.de

Thank you very much for your attention!

