Direct bioautography with subsequent DART-MS

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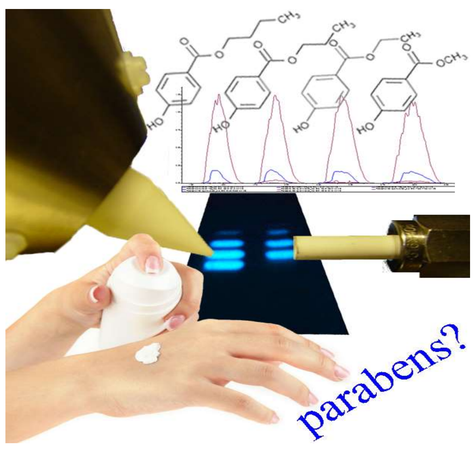
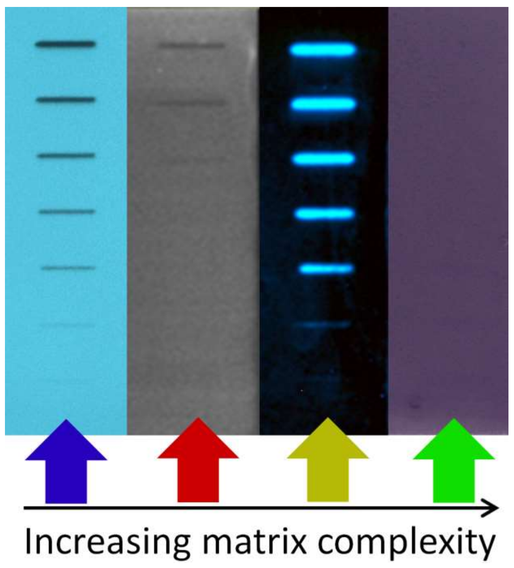


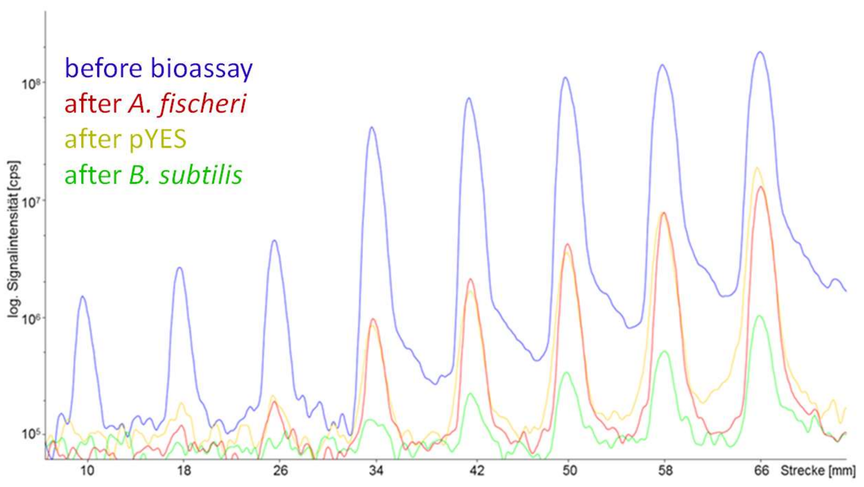
Highlights

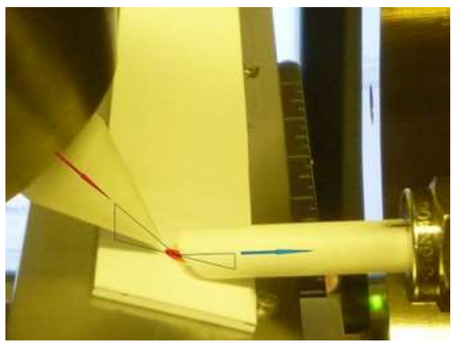
- *1th step: Direct bioautography (DB) to screen for bioactive compounds in complex samples*
- *2nd step: Matrix discriminating desorption-based mass spectrometry (HPTLC-DB-DART-MS)*
- *Characterization or quantification in one MS scan along a track or substance window*
- *Time-saving approach to evaluate bioactive characteristics and mass spectrometric information*



Influence of different bioassay media on scanning DART-MS?

- ✓ *Applied paraben standards (3-960 ng/band) quantitatively recorded via modified DART-MS [1, 2]*
- ✓ *Bioassay-dependent MS signal for Aliivibrio fischeri [3], planar yeast estrogen screen (pYES) [4] and Bacillus subtilis [5]: decreased with increasing matrix complexity!*

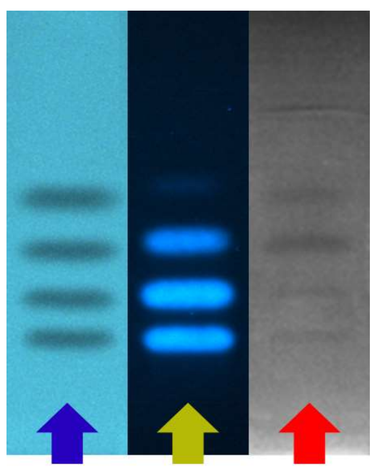


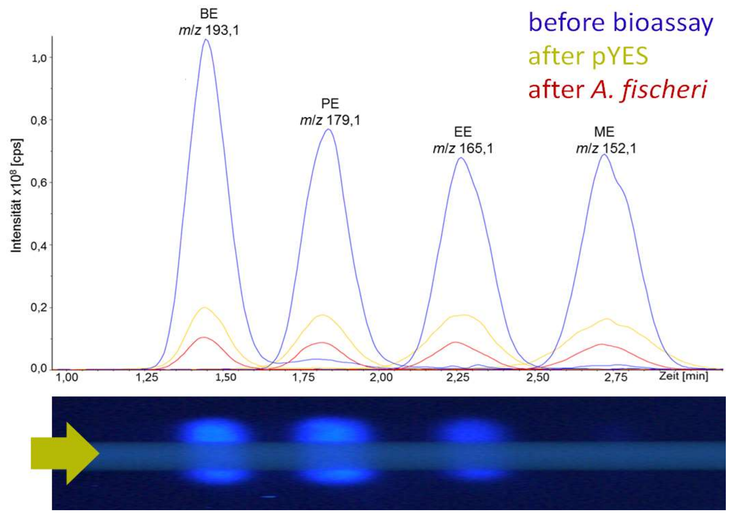


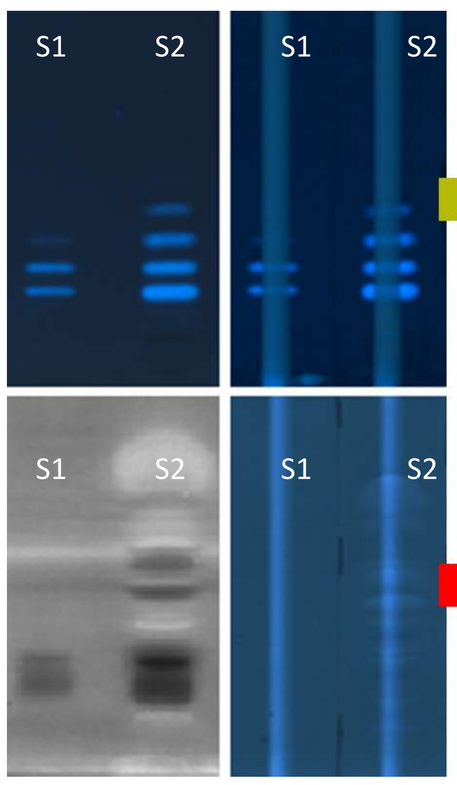
MS signal decay after DB ?

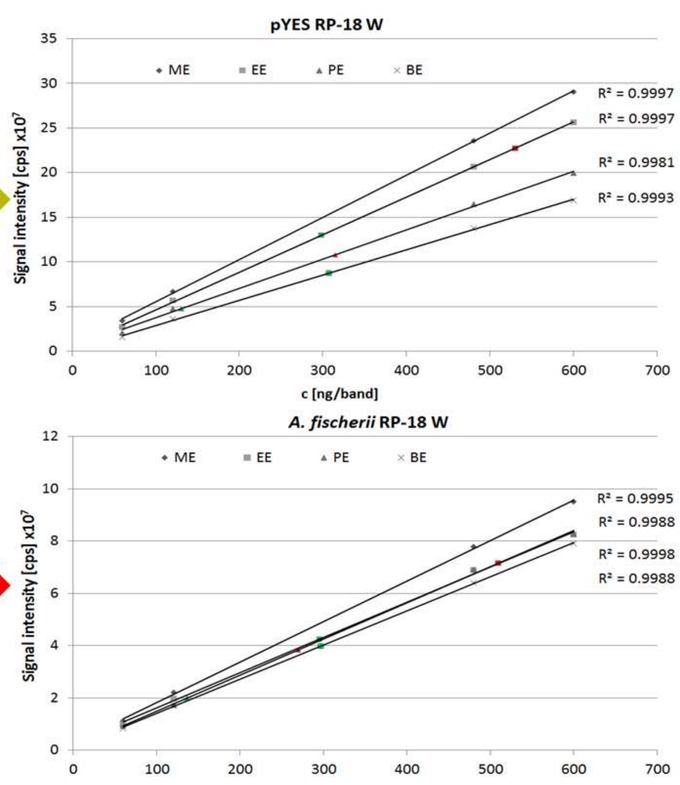
- ✓ *Separated paraben standards (each 600 ng/band) followed by DB with pYES and A. fischeri*
- ✓ *MS detection of the parabens via EIC chromatograms still sufficient for quantification!*

	Signal decay [%]	
	A. fischeri	pYES
ME	88	65
EE	89	67
PE	90	76
BE	91	81









Why DART-MS scanning after DB?

- ✓ *Results for bioactivity and MS of the same zone*
- ✓ *Reliable quantitation with a mean %RSD of 4.6% on normal and reversed phase layers*
- ✓ *Discriminating DART-MS: reduced contamination of the MS system and reduced ion suppression by the bioassay medium compared to ESI-MS*
- ✓ *Quantification by MS is not dependent on separation performance or zone shape after DB*

		Amount in sample [mg/100g]						
		Sample 1			Sample 2			
		ME	EE	PE	ME	EE	PE	BE
without BioAssay	NP	103	56	30	165	75	37	65
	RP	97	59	34	147	69	30	67
A. fischeri	NP	96	51	27	173	69	24	53
	RP	101	51	27	157	59	27	59
pYES	RP	111	53	31	170	60	26	62

References [1]T. Häbe, G. Morlock, Rapid Commun. Mass Spectrom. 29 (2015) 474. [2]T. Häbe, G. Morlock, Rapid Commun. Mass Spectrom. 30 (2016) 321. [3]S. Krüger, M. Mirgos, G. Morlock, J. Chromatogr. A 1426 (2015) 209. [4]M. Jamshidi-Aidji, G. Morlock, J. Chromatogr. A 1420 (2015) 110. [5]I. Klingelhöfer, G. Morlock, J. Chromatogr. A 1360 (2014) 288.

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