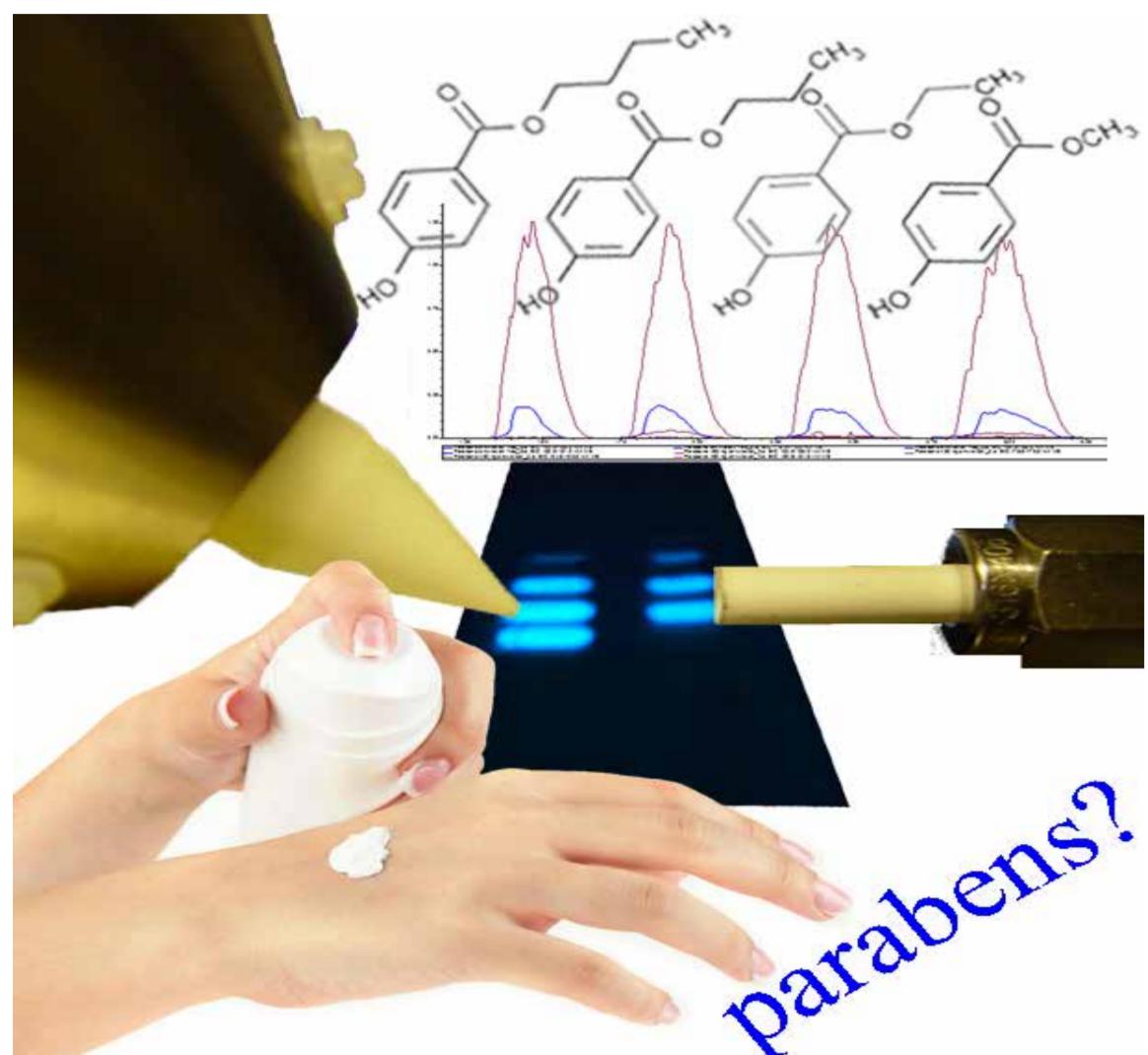


Direct bioautography directly combined with mass spectrometry

T.T. Häbe, M. Jamshidi-Aidji, J. Macho, G.E. Morlock

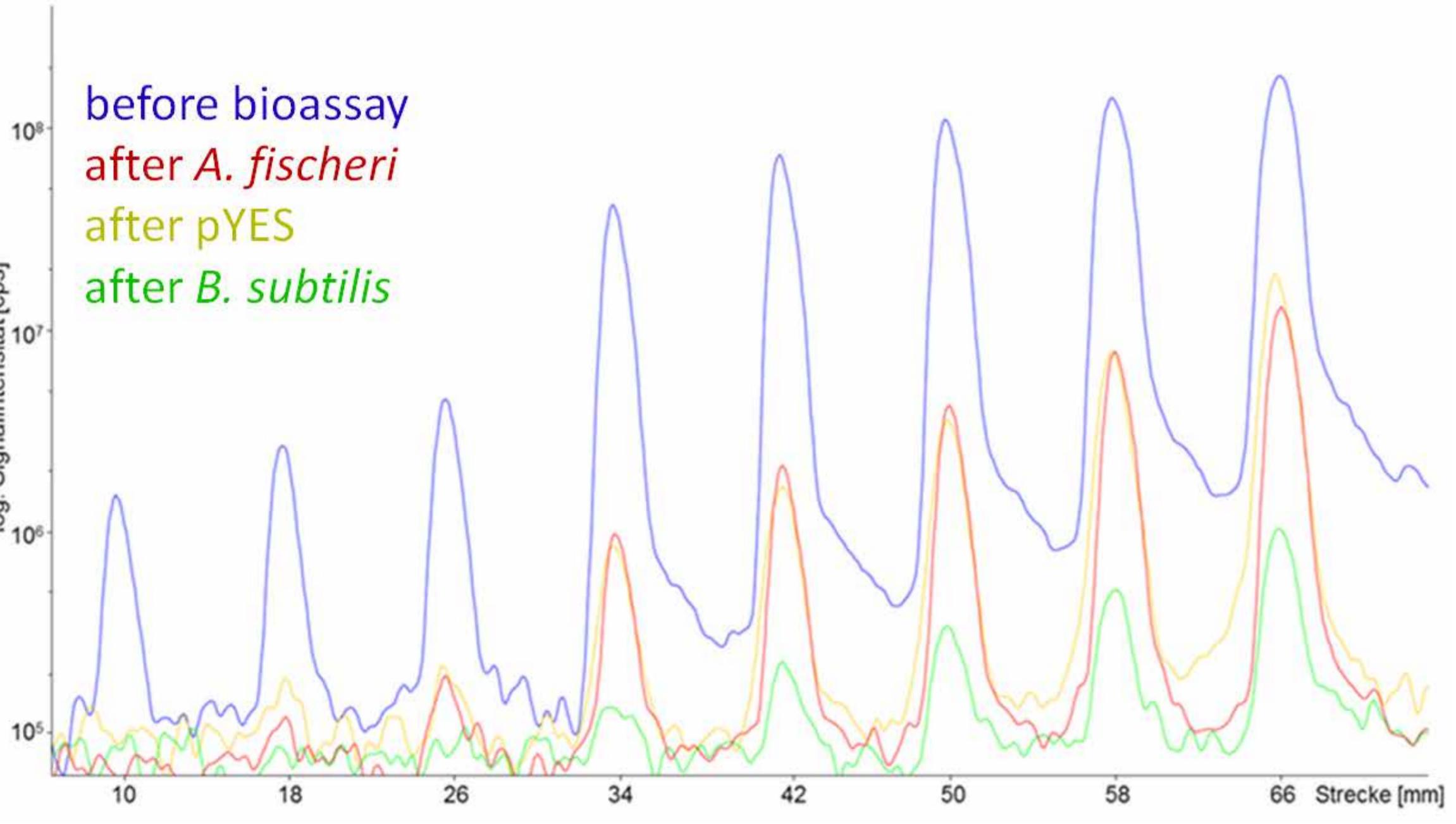
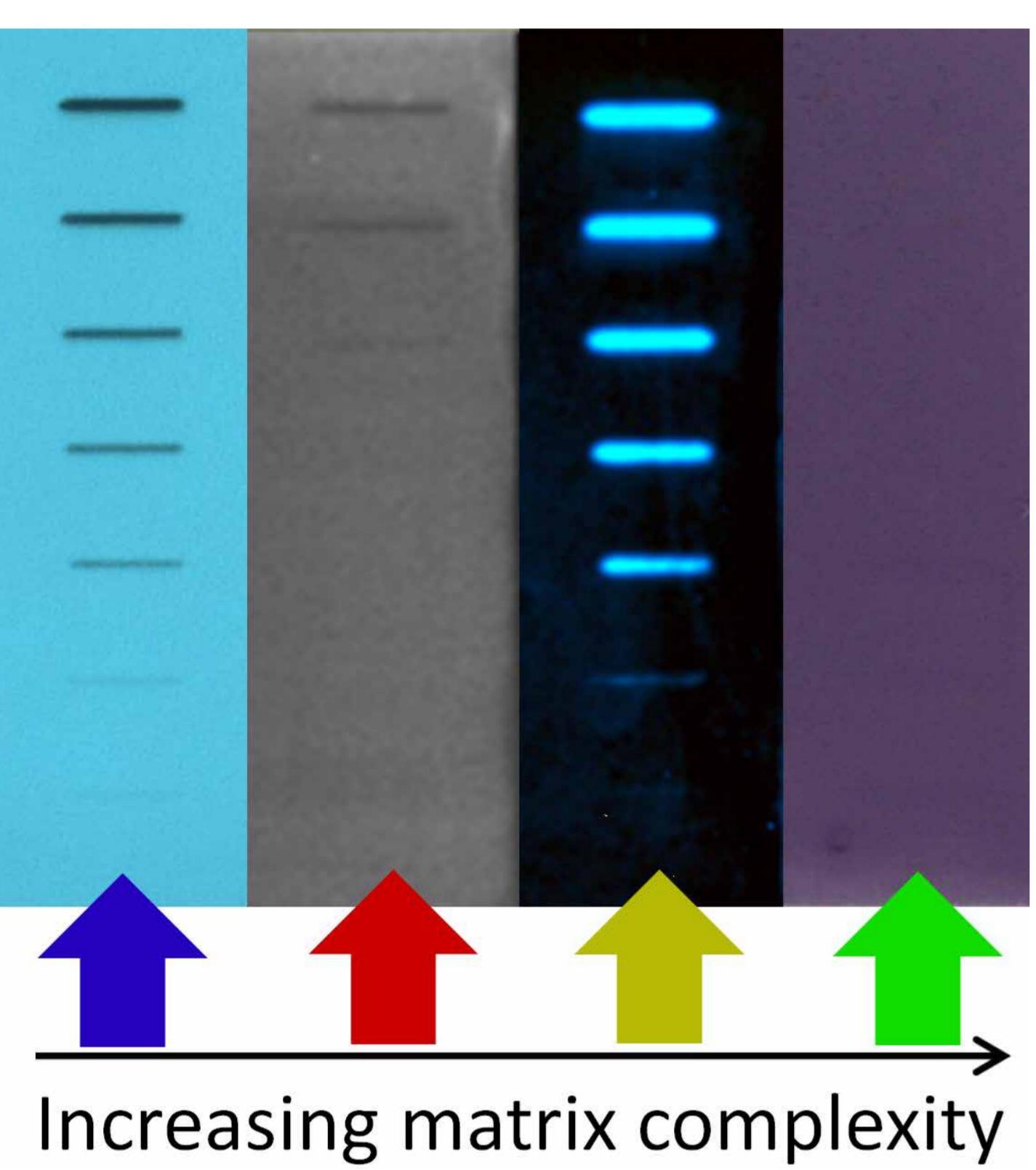
Justus Liebig University Giessen



parabens?

Highlights

- 1st step: Direct bioautography (DB) to screen for bioactive compounds in complex samples
- 2nd step: Matrix-discriminating desorption-based mass spectrometry from same plate (DB-DART-MS)
- Characterization or quantitation in one MS scan along a track or substance window
- Time-saving approach to evaluate bioactivity and mass spectrometric information



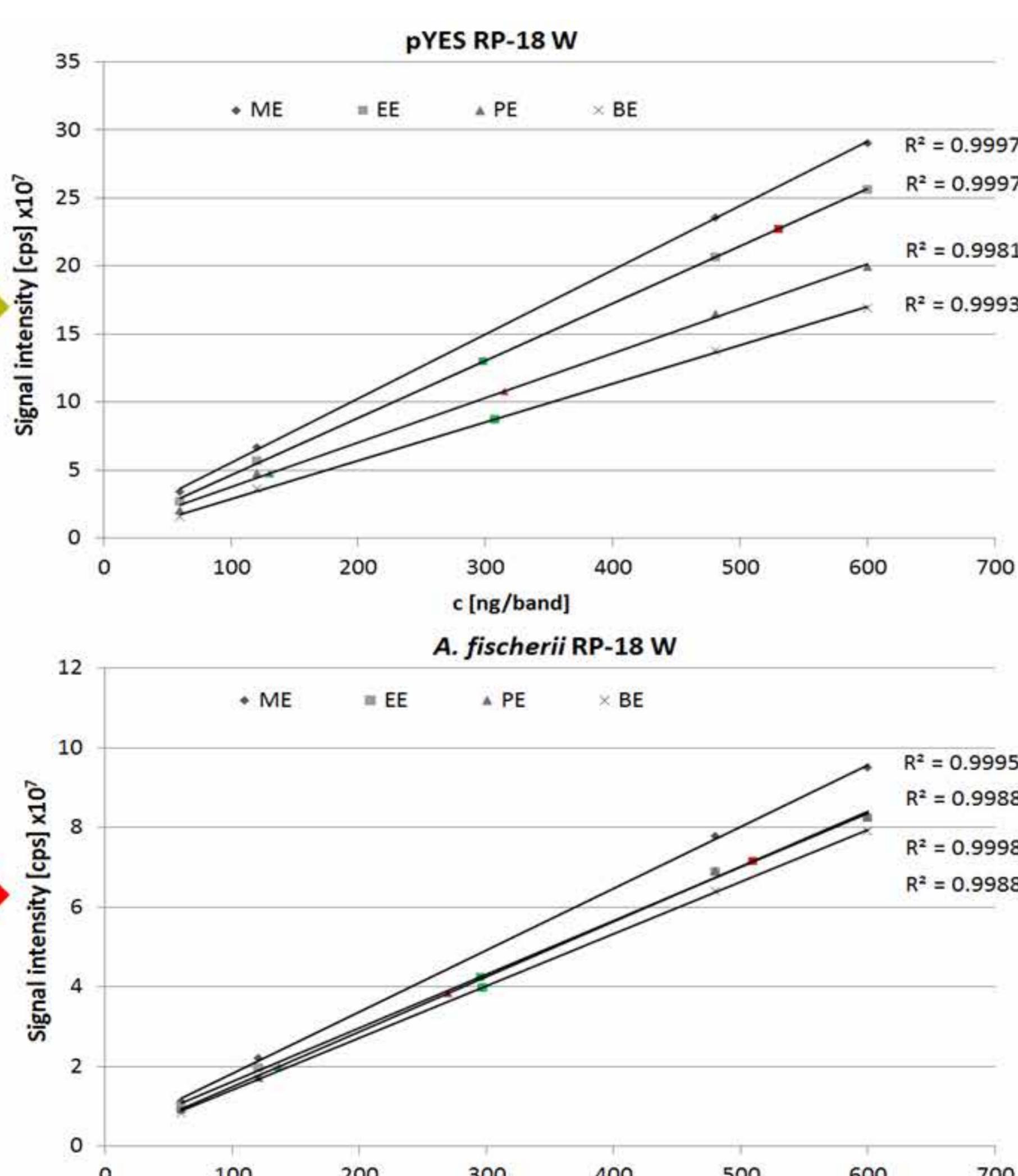
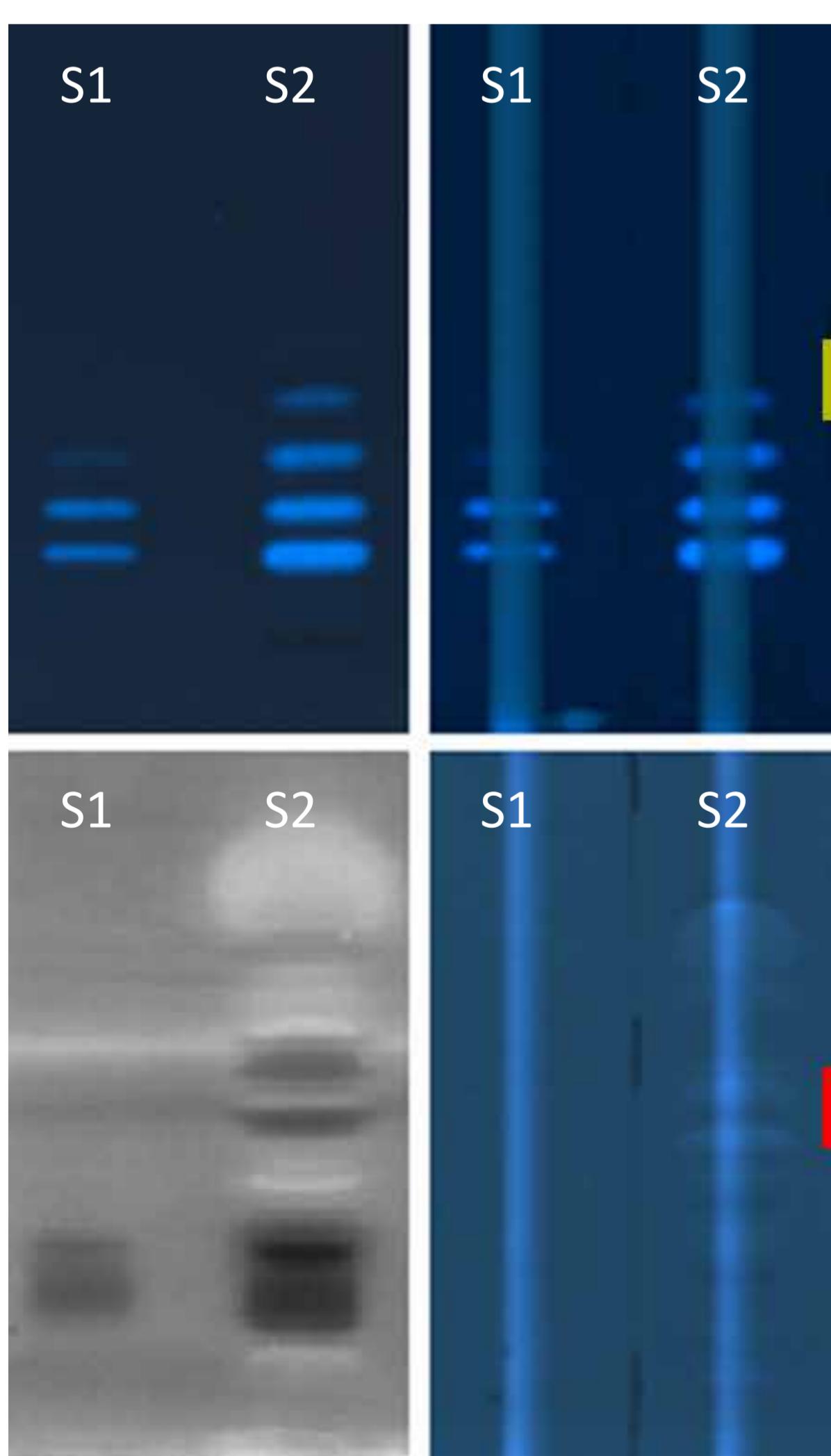
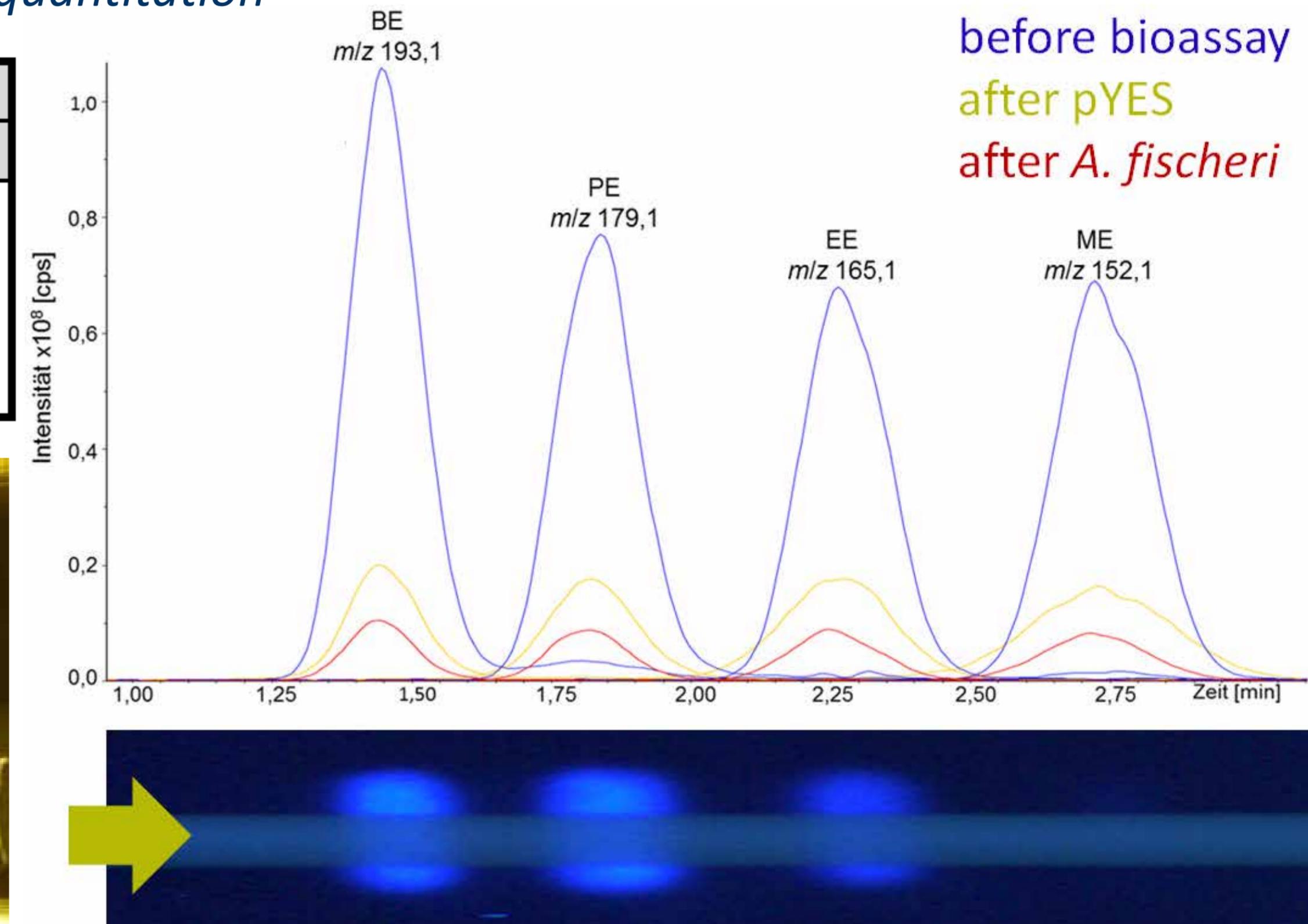
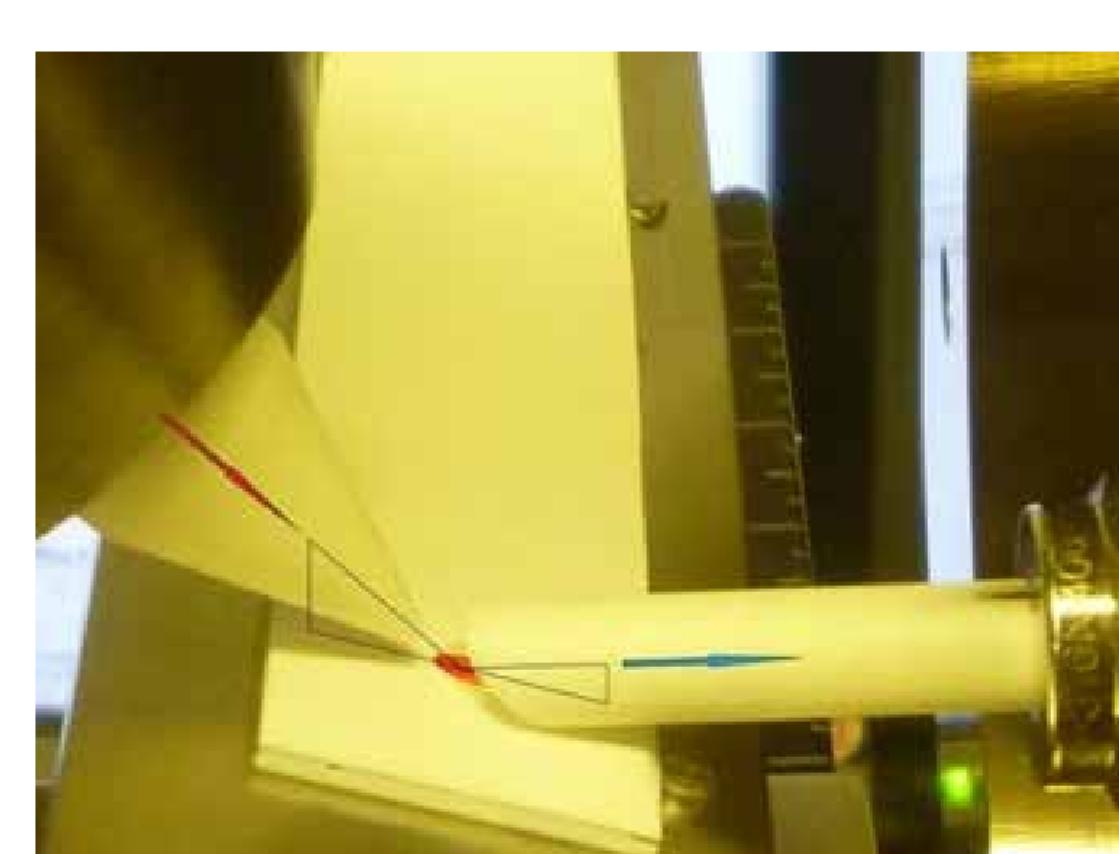
Influence of different bioassay media on scanning DART-MS?

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

Degree of MS signal decay after DB?

- ✓ Separated parabens (each 600 ng/band)
- ✓ Followed by DB with *pYES* and *A. fischeri*
- ✓ MS detection and selectivity via EIC chromatograms
- ✓ Sufficient detectability for quantitation

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



Why DART-MS scanning after DB?

- ✓ Results for bioactivity and MS obtained from the same zone
- ✓ Quantitation by DB-DART-MS (EIC) is independently on separation performance or zone shape
- ✓ Reliable DB-DART-MS quantitation with a mean deviation (%RSD) of 4.6% between *A. fischeri* and *pYES* bioassays (on RP phases)
- ✓ Advantageous discrimination through DART-MS scan: reduced contamination of the MS system by background/matrix/bioassay signals and thus less ion suppression compared to DB-ESI-MS



	Amount in sample [mg/100g]			
	Sample 1		Sample 2	
	ME	EE	PE	BE
without bioassay	NP	103	56	30
	RP	97	59	34
<i>A. fischeri</i>	NP	96	51	27
	RP	101	51	27
<i>pYES</i>	RP	111	53	31

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