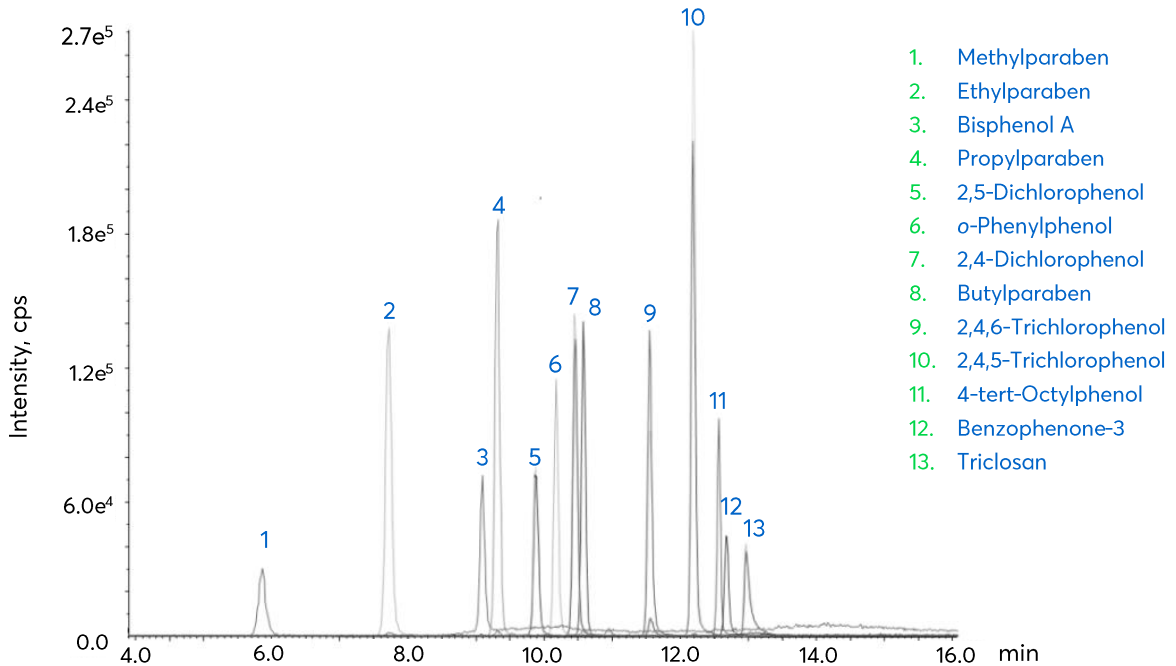


Environmental Phenols by LC-MS/MS



- 1. Methylparaben
- 2. Ethylparaben
- 3. Bisphenol A
- 4. Propylparaben
- 5. 2,5-Dichlorophenol
- 6. o-Phenylphenol
- 7. 2,4-Dichlorophenol
- 8. Butylparaben
- 9. 2,4,6-Trichlorophenol
- 10. 2,4,5-Trichlorophenol
- 11. 4-tert-Octylphenol
- 12. Benzophenone-3
- 13. Triclosan

Method Details

CONDITIONS

Column: Avantor® ACE® Excel® 3 C18-PFP

Particle Size: 3 µm

Dimensions: 100 x 4.6 mm

Mobile Phase: A: H₂O
B: MeOH

Gradient:

| Time (mins) | % B |
|-------------|-----|
| 0 | 60 |
| 2 | 60 |
| 10 | 100 |
| 15 | 100 |
| 15.1 | 60 |

Flow Rate: 0.5 mL/min

Injection: 10 µL

Detection: Sciex 5500 QTRAP MS
APCI in negative MRM mode
Curtain gas (N₂): 20 psi, Heated ion source gas: 30 psi,
Heated gas temperature: 450 °C, Nebuliser current: -3.5 µA

Sample: The chromatogram shows the separation of 13 phenols from a standard mixture in solvent. This method was developed to measure environmental phenols in human urine. Glucuronidated and sulphated metabolites were deconjugated by enzymatic hydrolysis and purified by SPE using C18 cartridges.



MRM TRANSITIONS

| Peak | Analyte | Transitions (m/z) | |
|------|-----------------------|-------------------|--------------|
| | | Quantifier | Confirmatory |
| 1 | Methylparaben | 151 > 92 | 151 > 136 |
| 2 | Ethylparaben | 165 > 92 | 165 > 137 |
| 3 | Bisphenol A | 227 > 133 | 227 > 212 |
| 4 | Propylparaben | 176 > 92 | 179 > 136 |
| 5 | 2,5-Dichlorophenol | 161 > 125 | 125 > 100 |
| 6 | o-Phenylphenol | 169 > 115 | 169 > 141 |
| 7 | 2,4-Dichlorophenol | 161 > 125 | 163 > 125 |
| 8 | Butylparaben | 193 > 92 | 193 > 136 |
| 9 | 2,4,6-Trichlorophenol | 195 > 159 | 197 > 161 |
| 10 | 2,4,5-Trichlorophenol | 195 > 159 | 197 > 161 |
| 11 | 4-tert-Octylphenol | 205 > 133 | n/a |
| 12 | Benzophenone-3 | 227 > 183 | 227 > 211 |
| 13 | Triclosan | 161 > 125 | 287 > 142 |

ORDERING TABLE

| Product | Details | Size | Part Number |
|--------------------------------|-------------------------------------|--------------|----------------|
| Avantor® ACE® Excel® 3 C18-PFP | HPLC Column | 100 x 4.6 mm | EXL-1110-1046U |
| Methanol | VWR HiPerSolv CHROMANORM® for LC-MS | 2.5 L | 83638.320 |
| Water | VWR HiPerSolv CHROMANORM® for LC-MS | 2.5 L | 83645.320 |

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