Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Detecting a wide range of environmental contaminants in human blood samples—combining QuEChERS with LC-MS and GC-MS methods

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<table>
<thead>
<tr>
<th>Compound name</th>
<th>Compound group</th>
<th>CAS No</th>
<th>Molecular formula</th>
<th>log K\textsubscript{OW}</th>
<th>Henry constant</th>
<th>pK\textsubscript{a} values</th>
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<tr>
<td>2,4-toluene diisocyanate</td>
<td>allergenic substance, chemical intermediate</td>
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<td>5-chloro-2-methyl-4-isothiazolin-3-one (methylchloroisothiazolinone)</td>
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<td>26172-55-4</td>
<td>C\textsubscript{6}H\textsubscript{5}ClN\textsubscript{2}S</td>
<td>-0.34</td>
<td>3.6E\textsuperscript{-08}</td>
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<td>citronellal</td>
<td>allergenic substance, fragrance, cosmetic ingredient</td>
<td>106-23-0</td>
<td>C\textsubscript{10}H\textsubscript{18}O</td>
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<td>resorcinol</td>
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<td>4,4’-thiodianiline</td>
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<td>7.3E\textsuperscript{-11}</td>
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Perfluorinated compounds (PFCs): Perfluorobutanoic acid, perfluorooctanoic acid, perfluorotetradecanoic acid, perfluorooctane sulfonic acid, 2-N-methylperfluorooctanesulfonamide (MeFOSA), perfluorooctyl phosphonic acid (C8-PEPA), 8:2 fluorotelomer alcohol (8:2 FTOH), and 10:2 fluorotelomer alcohol (10:2 FTOH) are listed with their respective CAS numbers and molecular formulas.
<table>
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<th>Substance</th>
<th>Description</th>
<th>CAS Number</th>
<th>Molecular Formula</th>
<th>pK_a</th>
<th>Prediction</th>
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<tr>
<td>hydroxybenzamide (tetrachlorosalicylanilide)</td>
<td>quaternary ammonium compound (QAC), biocide, allergenic substance</td>
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<td>C_{16}H_{16}Cl_{3}N_{4}</td>
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<td>C_{21}H_{38}N</td>
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<td>4.8E-13</td>
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<td>trimethyloctyl-ammonium bromide (trimethylQUAT)</td>
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<td>C_{18}H_{26}O_{3}</td>
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a calculated using EPI Suite (www.epa.gov/oppt/exposure/pubs/episuitedl.htm); b calculated using Calculator Plugins, Instant JChem 2012, ChemAxon (www.chemaxon.com), only given for 0 < pK_a < 14; a is the pK_a value for the corresponding acid; b not calculated, as predictions for highly fluorinated compounds have been of debate, thus latest estimations based on measurements by Vierke et al. are listed here [2].
<table>
<thead>
<tr>
<th>compound name</th>
<th>monoisotopic mass</th>
<th>final method</th>
<th>HRMS target m/z</th>
<th>QTrap -MRM</th>
<th>blood spike std [µg/mL]</th>
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<td>n.d.</td>
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<td>IS Spike Std [µg/mL]</td>
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<td>n.d.</td>
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**internal standards (IS)**

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<th>Compound</th>
<th>Monoisotopic Mass</th>
<th>Final Method</th>
<th>HRMS Target m/z</th>
<th>QTrap -MRM</th>
<th>IS Spike Std [µg/mL]</th>
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Table S3 MRM transitions, instrument parameters, instrumental detection limits (IDL), linearity and method quantification limits (MQL) for the target compounds during LC-MS/MS analysis (QTrap 6500 instrument), compounds in brackets were not included in the final method; n.i. = not included in the final method

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<th>$Q_1$ (Da) &gt; $Q_3$ (Da)</th>
<th>DP (volts)</th>
<th>CE (volts)</th>
<th>CXP (volts)</th>
<th>IDL [ng/mL extract]</th>
<th>Linear range of calibration</th>
<th>Correlation coefficient of calibration ($r^2$)</th>
<th>MQL (ng/mL blood)</th>
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<td></td>
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<td>175.0 &gt; 77.0</td>
<td>161</td>
<td>37</td>
<td>10</td>
<td>n.i.</td>
<td>n.i.</td>
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DP: declustering potential; CE: collision energy; CXP: collision cell exit potential
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<th>quantifier</th>
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<th>Correlation coefficient ($r^2$) of calibration</th>
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**Internal standards**

<p>| tonalide-d&lt;sub&gt;3&lt;/sub&gt;          | GC    | 261       | 246        | 21.3     |                   |                             |                                               |                  |</p>
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RT: retention time; IDL: instrument detection limit; MQL: method quantification limit; blank: detection in pig blood extract
Table S5 Target analytes detected in the three method blanks. Concentrations given in ng/mL (blood equivalent), standard deviation in brackets

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<td>0.11 (0.009)</td>
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<td>0.09 (0.043)</td>
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<td>TCEP</td>
<td>nd</td>
<td>0.07 (0.009)</td>
<td>na</td>
</tr>
<tr>
<td>PFOA</td>
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<td>tetrachlorosalicylanilide</td>
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<td>0.067 (0.020)</td>
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</tr>
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<td>na</td>
<td>1.5 (0.08)</td>
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<td>na</td>
<td>na</td>
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nd: not detected; na: not analysed
Fig. S1 Total ion chromatograms of pig blood extracts after LLE (liquid-liquid extraction) and dSPE (dispersive solid phase extraction) analysed by (A) LC-HRMS ESI positive, (B) LC-HRMS ESI negative, and (C) GC-EI-MS
Fig. S2 Relative recoveries compared to a matrix spike of the LC-MS target analytes. Analytes were spiked at 3 different concentrations into pig blood followed by LLE extraction. Bars represent the minimum and maximum values, n=3 for 50 ng/mL, n=2 for 2 and 10 ng/mL. MeFOSA has been determined in a separate experiment only for the 10 and 50 ng/mL levels, n=1, due to low concentrations of the reference standard.
Fig. S3 Relative recoveries compared to a matrix spike of the GC-MS target analytes. Analytes were spiked at 3 different concentrations into pig blood followed by LLE extraction. Bars represent the minimum and maximum values, n=3 for 50 ng/mL, n=2 for 2 and 10 ng/mL. BDE 47 and BDE 99 were determined in a separate experiment only for the 10 and 50 ng/mL levels, n=1, due to low concentrations of the reference standard.
**Fig. S4** Absolute recoveries of GC-MS target analytes comparing the spiked pig blood with two spiked human blood samples (W17 and M14). Bars represent the minimum and maximum values for pig blood. 4-methylanisole could not be evaluated during the human blood analysis due to its early RT resulting in peaks cut by the set SIM window.
Fig. S5 Average absolute recoveries of internal standards spiked into the 16 human blood samples, comparing LC-MRM and LC-HRMS-full scan analysis. The whiskers represent minimum and maximum values.
Fig. S6 Average absolute recoveries of two spiked human blood samples comparing MRM and HRMS-full scan analysis
Fig. S7 Selected ion chromatograms of PFCAs detected in sample M14

References