

Electronic Supplementary Information

Autarkic desorption electrospray ionization source for on-site analysis of consumer goods

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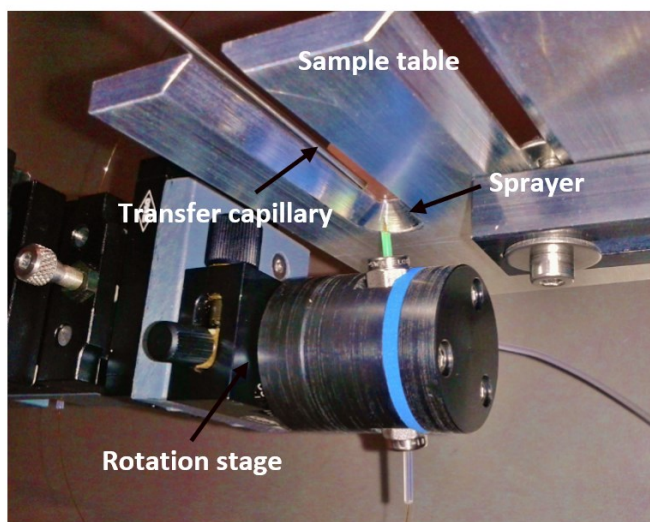


Figure S-1. DESI sprayer mounted on a rotation stage and installed under a cleft sample table. This setup was used to investigate the desorption and ionization efficiency using this inverse sprayer geometry.

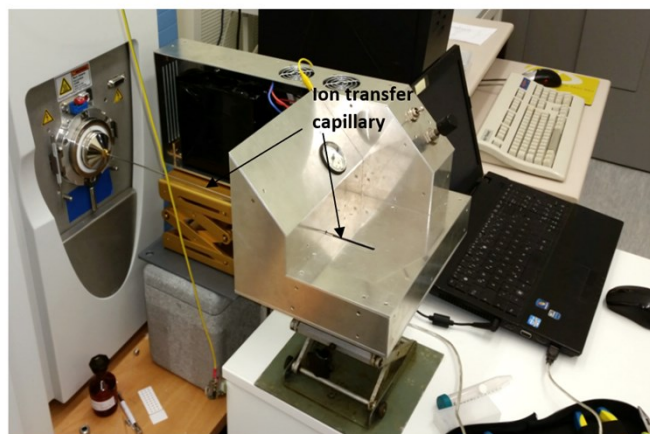


Figure S-2. Setup for the measurements with the autarkic DESI source coupled to an orbital-trapping mass spectrometer (Exactive Orbitrap, Thermo Fisher Scientific).

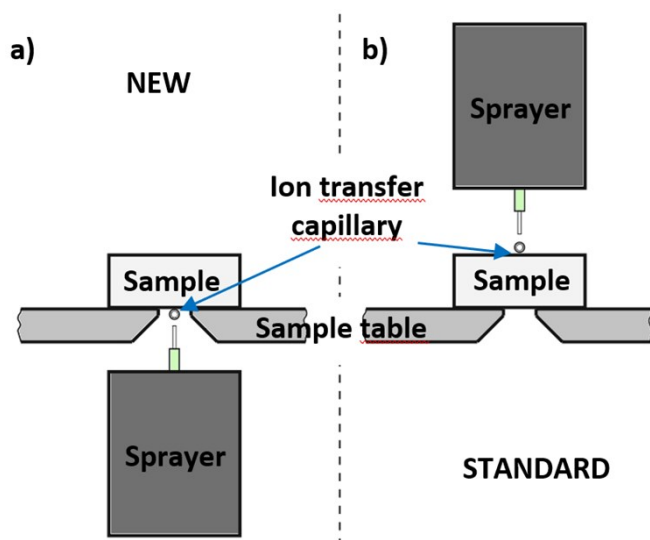


Figure S-3. a) New sprayer arrangement and b) conventional DESI setup. Direction of view is along the ion transfer capillary.

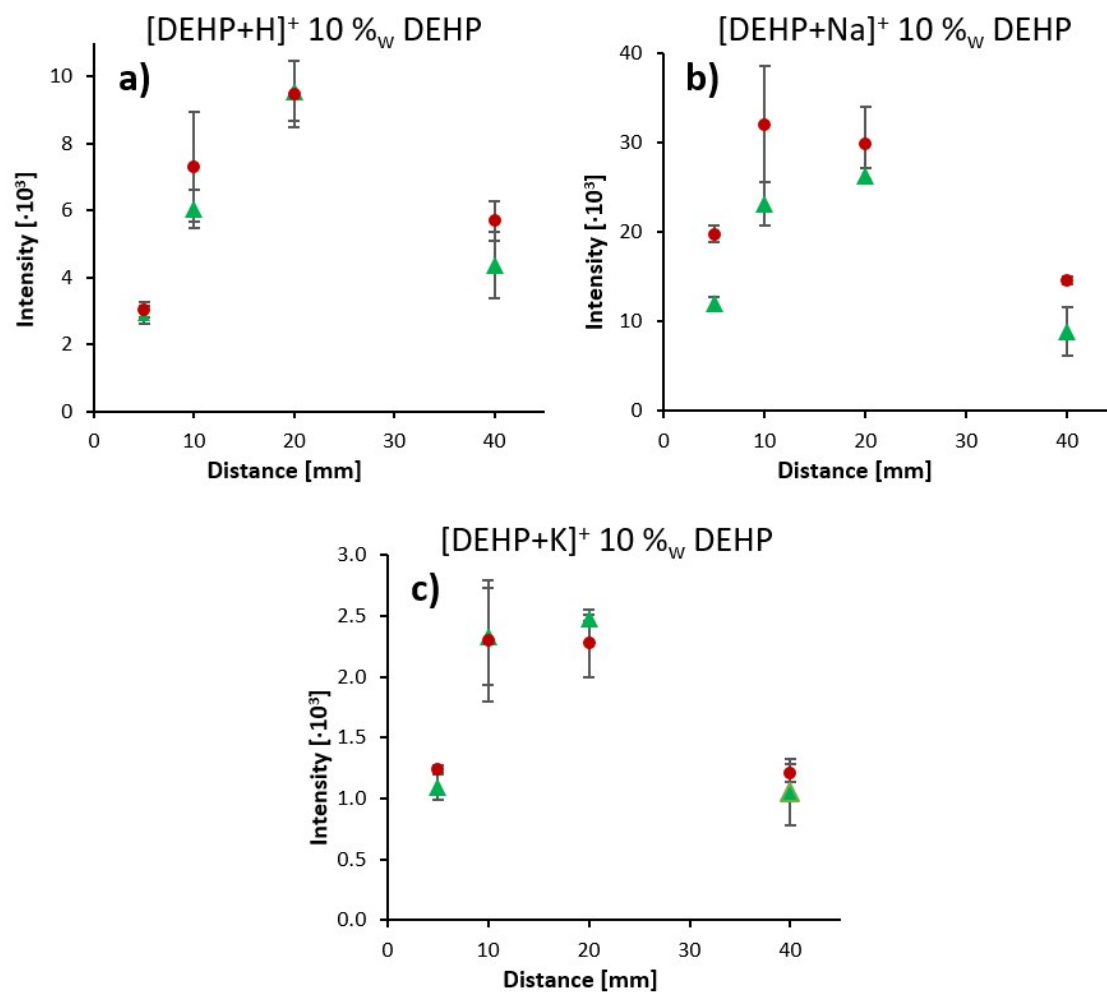


Figure S-4. Comparison of the signal intensities of a) $[\text{DEHP}+\text{H}]^+$, b) $[\text{DEHP}+\text{Na}]^+$ and c) $[\text{DEHP}+\text{K}]^+$ for the DESI MS measurements of a plastisol pill containing 10 %_w DEHP with the new (dots) and conventional sprayer geometry (triangles) as a function of the sprayer-to-ion transfer capillary distance.

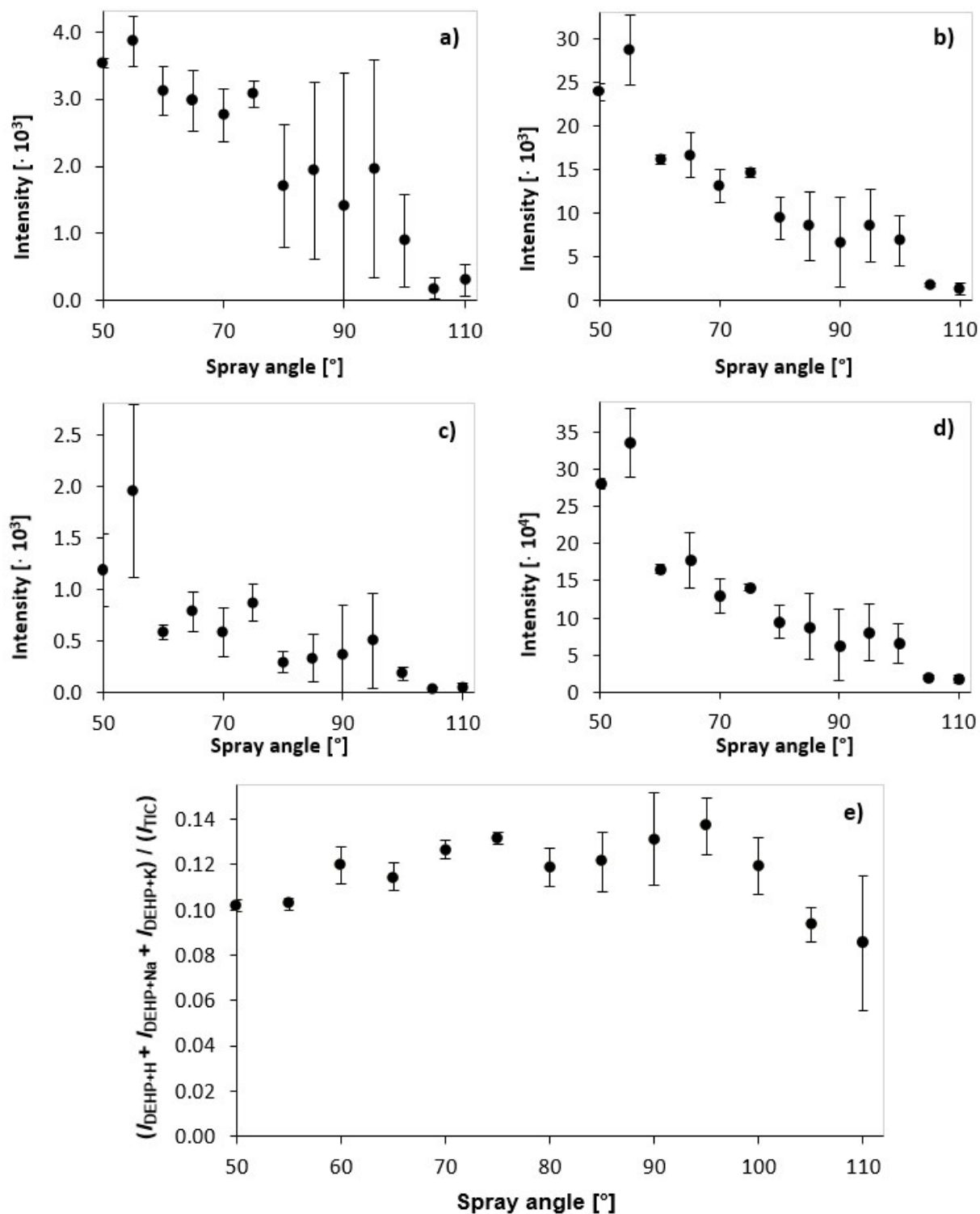


Figure S-5. Signal intensities obtained with the new sprayer geometry for a plastisol pill with 10 %_w DEHP as a function of the sample-to-sprayer-angle. a) [DEHP+H]⁺, b) [DEHP+Na]⁺, c) [DEHP+K]⁺ and d) total ion current. e) shows the dependency of the chemical noise to the sample-to-sprayer angle. Measured was the plastisol pill with a sprayer-to-ion-transfer-capillary distance of 5 mm.

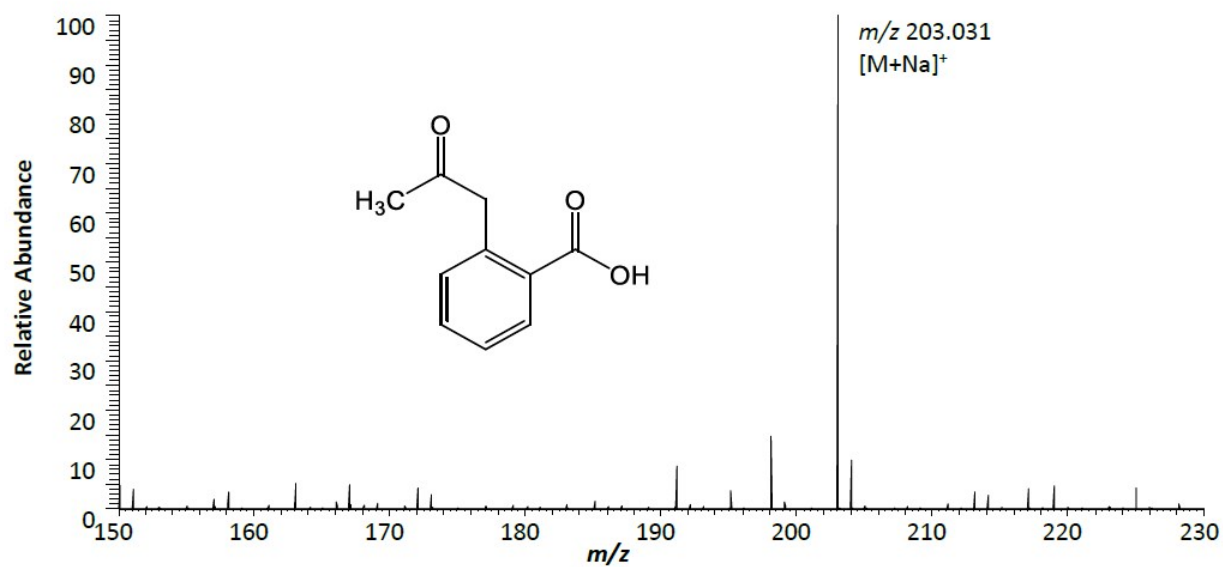


Figure S-6. DESI mass spectrum of an acetylsalicylic acid pill analyzed directly with the autarkic DESI source coupled to an orbital trapping mass spectrometer. The sodium adduct of the drug acetylsalicylic acid ($[M+Na]^+$, m/z 203.031) was detected with high signal intensity.

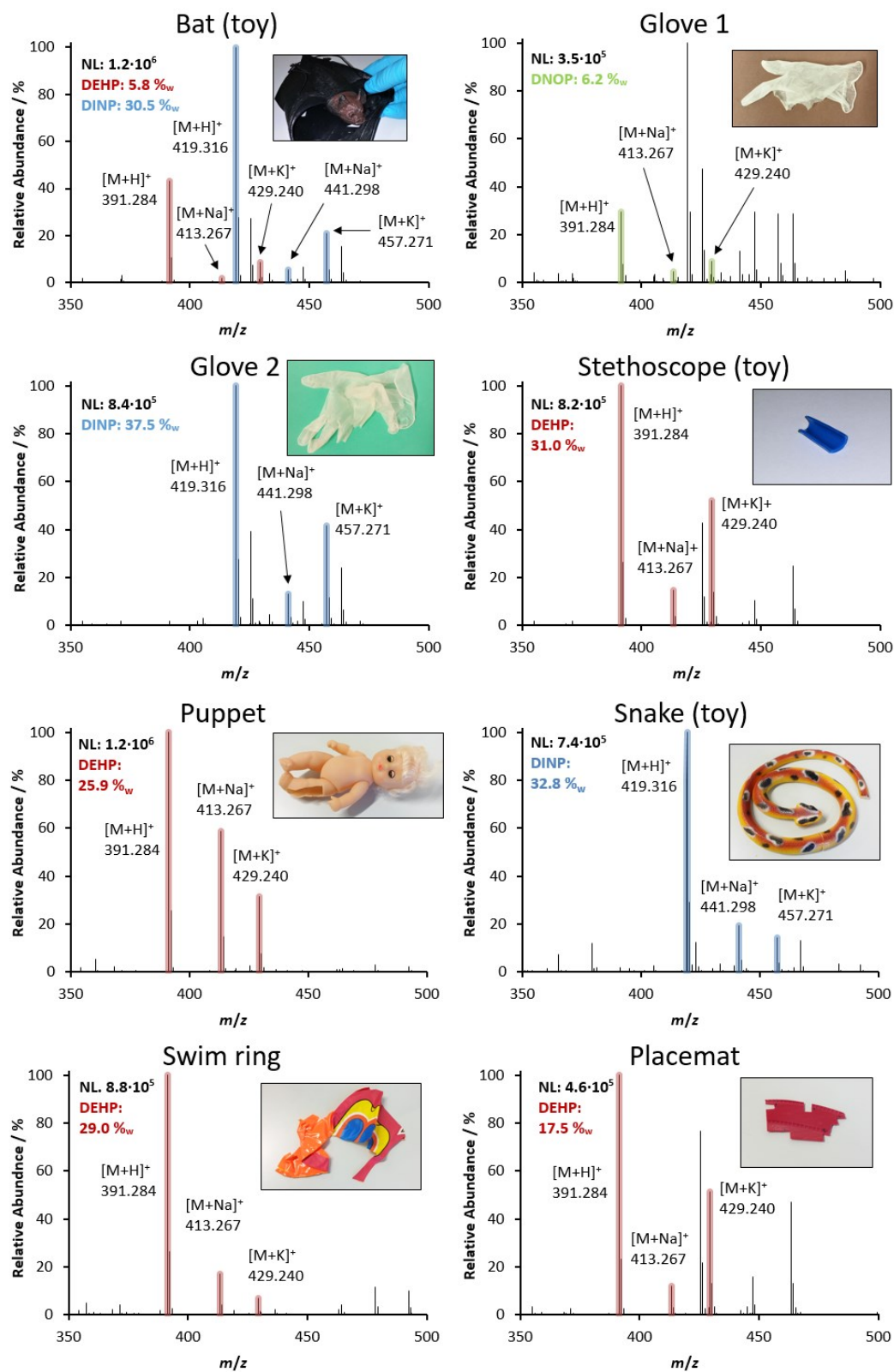


Figure S-7. DESI mass spectra of various sample objects which contain the phthalate-based plasticizers DEHP, DINP and DNOP, analyzed directly with the autarkic DESI source coupled to an orbital-trapping mass spectrometer.

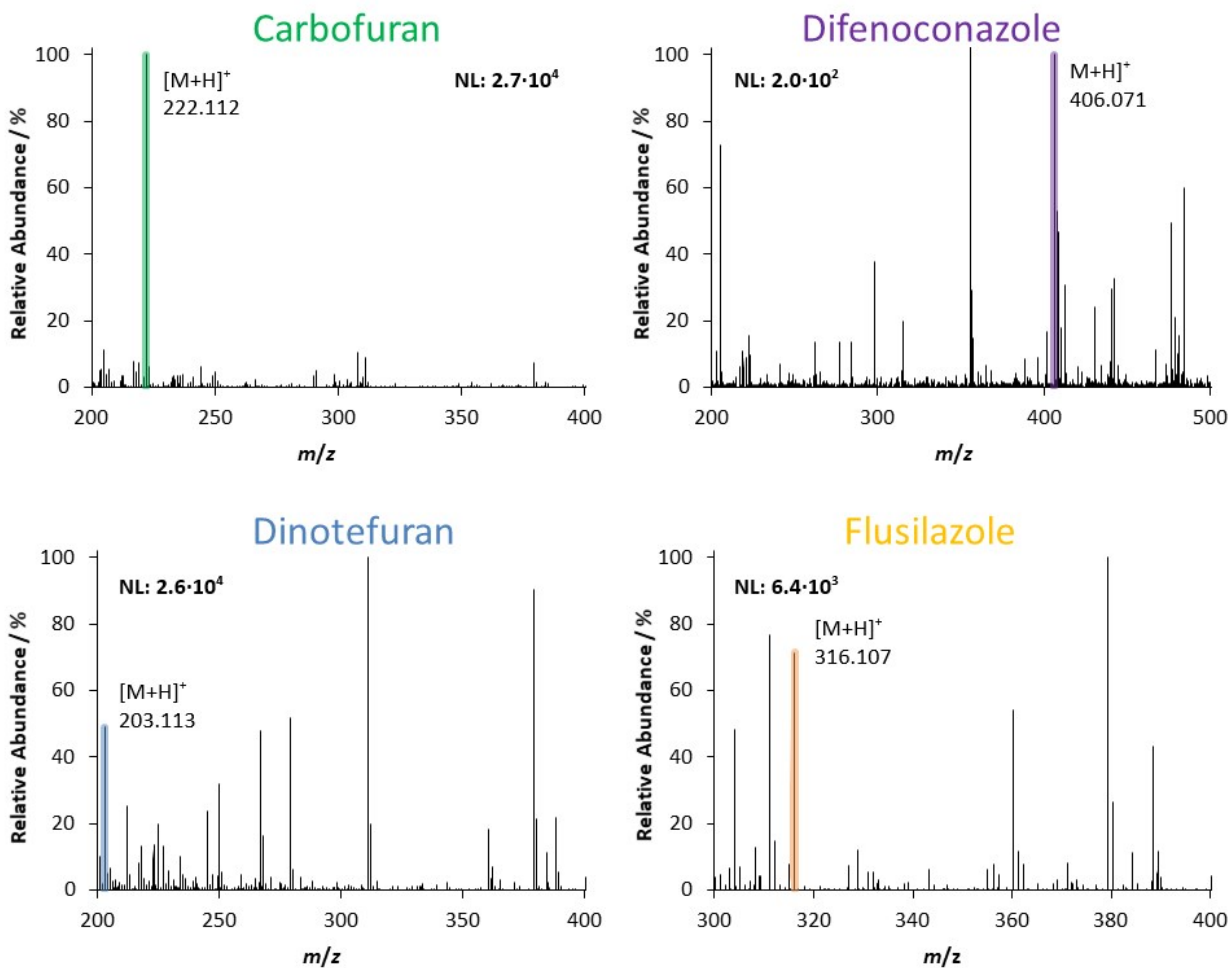


Figure S-8. DESI mass spectra of pesticides detected directly from a spiked apple peel at a concentration of 30 ng/cm² with the autarkic DESI source coupled to an orbital-trapping mass spectrometer. Shown are differential spectra of 20 consecutive spectra from the spiked apple peel and 20 spectra from untreated apple peel.

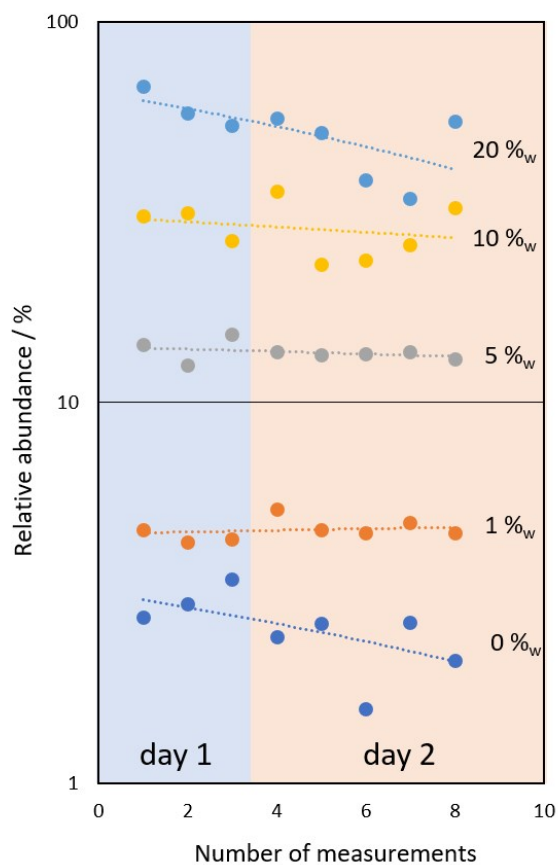


Figure S-9. Inter-day and intra-day reproducibility of calibration curves, obtained from the same set of DEHP plastisol pills. At day 1, three and at day 2, five technical replicates were measured. Shown is the TIC-normalized sum of DINP ions ($[M+H]^+$, $[M+Na]^+$, $[M+K]^+$) against measurement number.

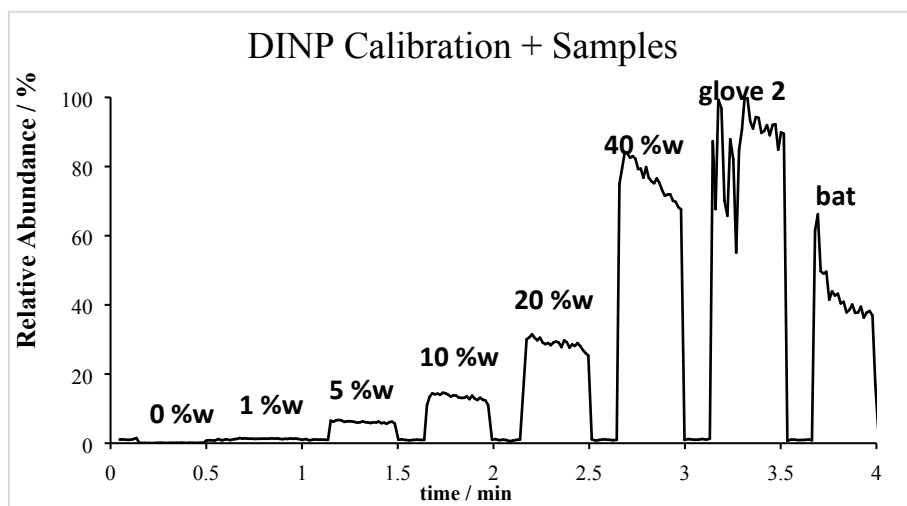


Figure S-10. Chromogram of a quantitative DESI measurement set. Six plastisol pills with DINP concentrations of 0 - 40 %_w and two real samples were analyzed. Shown is the TIC-normalized sum of DINP ions ($[M+H]^+$, $[M+Na]^+$, $[M+K]^+$) against measurement time. Each pill or sample was measured for 20 s, followed by 5 s for switching between samples.