

Supplementary Data

Trace Detection of Molecules Distributed across Surfaces using Mass Transfer and Large-Area Desorption Electrospray Ionization (DESI) Mass Spectrometry

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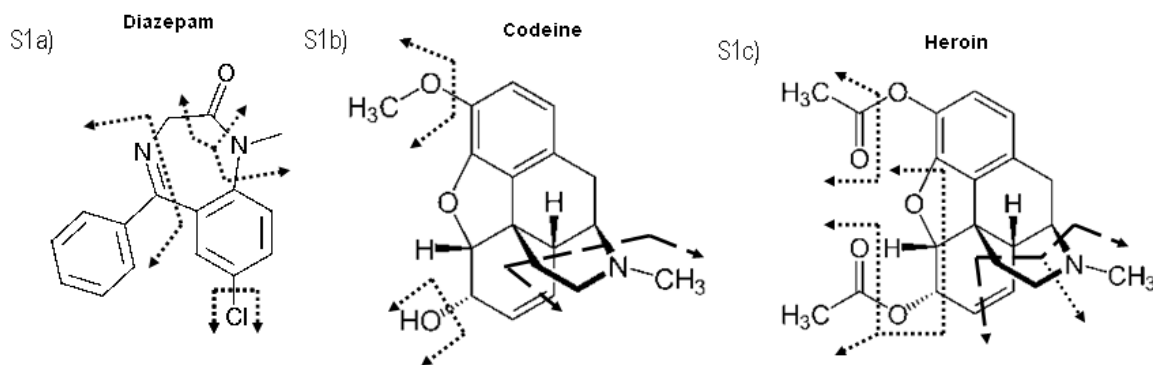
Summary

The supplementary material includes data on the limits of detection and MS/MS fragmentation processes for diazepam, codeine and heroin.

Table S1 Limits of detection for diazepam and codeine collected from a 10 cm² plastic surface using different wipe materials and examined in situ on the wipe

	<i>Diazepam</i>				<i>Codeine</i>			
Wipe	LOD (ng)	R^2	Slope (counts/ng)	Recovery (%)	LOD (ng)	R^2	Slope (counts/ng)	Recovery (%)
<i>DSA</i> [®] <i>cloth</i>	22	0.95	18	65	17	0.97	24	73
<i>Swiffer</i> [®] <i>duster</i>	35	0.91	10	69	23	0.92	16	68
<i>Swiffer</i> [®] <i>mop</i>	41	0.87	5.9	57	32	0.82	8.7	61

Scheme S1



Scheme S1: The product ion MS/MS spectrum of $[\text{diazepam}+\text{H}]^+$ (**Figure S1a**) shows typical fragment ions at m/z values of 257 $[\text{M}-\text{COH}]^+$, 240 $[[\text{M}-\text{COH}]-\text{NH}_3]^+$, 228 (opening of the 7-membered ring with loss of $-\text{CH}_3\text{NCO}$), 222 $[\text{M}-\text{COClH}]^+$, 182 $[\text{M}-\text{C}_7\text{H}_5\text{NH}]^+$, and 154 (loss of benzonitrile from $[\text{M}-\text{COH}]^+$). The corresponding data for $[\text{codeine}+\text{H}]^+$ produced fragment ions (**Figure S1b** at m/z values 282 $[\text{M}-\text{H}_2\text{O}+\text{H}]^+$ and m/z 243 $[\text{M}-\text{CH}_2\text{CHNHCH}_3\text{H}]^+$. The latter ion undergoes further dehydration and decarboxylation to yield the species at m/z 225 and m/z 215, respectively. Loss of CH_3OH from the ion at m/z 225 yields the fragment observed at m/z 183. Deacetylation at either the O-3 or O-5 position of $[\text{heroin}+\text{H}]^+$ (m/z 370) gives the ion at m/z 328 in MS^2 spectra (**Figure S1c**). The ion at m/z 268 $[\text{M}-\text{C}_4\text{H}_6\text{O}_3\text{H}]^+$ has multiple routes of formation that involve deacetylation, dehydration and loss of CH_3COOH . Loss of $-\text{CH}_3\text{NH}_2$ and $-\text{CH}_2\text{CHNHCH}_3$ from m/z 268 gives the fragments m/z 237 and 211, respectively. The ion at m/z 193 corresponds to loss of H_2O from m/z 211.