

# Supplemental Information

*for*

## Electrochemical detection of MDMA and 2C-B in ecstasy tablets using a selectivity enhancement strategy by *in-situ* derivatization

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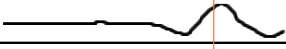
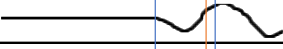
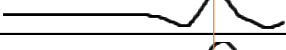
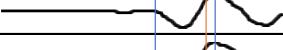
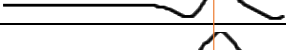
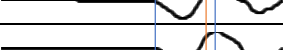
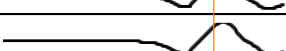
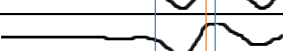


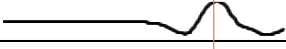
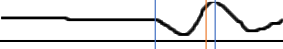
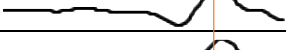
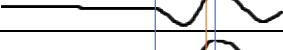

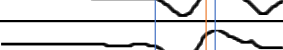
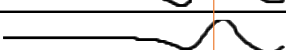
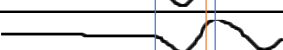
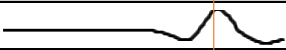
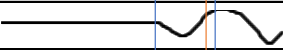
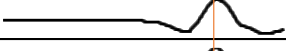
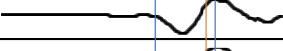
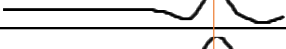


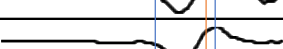
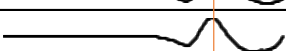

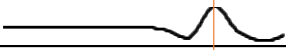
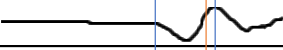
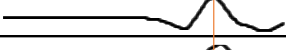
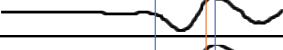
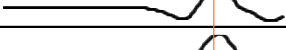
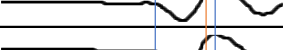

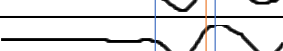
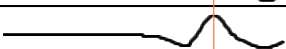
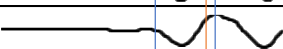
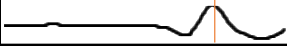
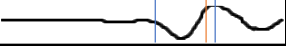
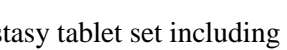
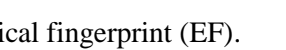






<b>Figure S1</b>	Picture of the ecstasy tablets selected for this study.
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**Figure S1.** Ecstasy tablets selected for this study. Tablets 1 to 40 contained MDMA, tablets 101 – 133 contained other substances. Main active ingredients are given in Tables 1 and S2. *Note that samples #15 and #103 are omitted.*

#	IDENTITY	MDMA SENSOR OUTPUT	MDMA SENSOR CURVE
1	MDMA	MDMA	
2	cocaine base	-	
3	cocaine HCl	-	
4	ketamine	-	
5	amphetamine	-	
6	methamphetamine	-	
7	heroin	-	
8	2C-B	MDMA	
9	sildenafil	-	
10	oxazepam	-	
11	flunitrazepam	-	
12	diazepam	-	
13	methylphenidate	-	
14	GHB	-	
15	4-FA	-	
16	2-FMA	-	
17	3-FMA	-	
18	4-FMA	-	
19	2-MEC	-	
20	3-MEC	-	
21	4-MEC	-	
22	2-MMC	-	
23	3-MMC	-	
24	4-MMC	-	
25	3,4-DMMC	-	
26	3-CMC	-	
27	4-CMC	-	
28	4-CEC	-	
29	pentedrone	-	
30	2,3-MDA	-	
31	3,4-MDA	MDMA	
32	2,3-MDMA	-	
33	3,4-MDEA	-	
34	methylone	MDMA	
35	ethylone	MDMA	
36	2,3-ethylone	MDMA	
37	2,3-methylone	-	
38	dimethylone	-	
39	pentylone	-	
40	5-APB	-	
41	6-APB	-	
42	alpha-PVP	-	
43	MDPV	-	
44	AM-2201	-	
45	5-F-APINACA	-	
46	mCPP	MDMA	
47	paracetamol	-	
48	caffeine	-	
49	levamisole	-	
50	lidocaine	-	
51	phenacetine	-	
52	procaine	-	
53	benzocaine	-	
54	mannitol	-	
55	lactose	-	
56	inositol	-	
57	vitamin C	-	
58	sugar	-	
59	glucose	-	
60	boric acid	-	
61	diltiazem	-	
62	promethazine	MDMA	
63	creamer	-	
64	starch	-	
65	aspirin	-	
66	paracetamol:caffeine	-	
67	levamisole:lidocaine	-	
68	levamisole:paracetamol:lidocaine	-	
69	levamisole:phenacetine	-	
70	phenacetine:lidocaine	-	
71	phenacetine:procaine	-	
72	levamisole:phenacetine:procaine	-	
73	paracetamol:phenacetine	-	
74	cutting agent mix	-	

**Table S1.** Results of the MDMA electrochemical sensor including the obtained electrochemical fingerprint (EF) on drugs-of-abuse, common pharmaceuticals, NPS, excipients and adulterants. Red line indicates the 1.11 V peak diagnostic for MDMA.

TABLET ID	IDENTITY	COLOR	WEIGHT (mg)	MDMA SENSOR OUTPUT	MDMA SENSOR CURVE	MDMA/2C-B SENSOR OUTPUT	MDMA/2C-B SENSOR CURVE
1	MDMA	grey	512	MDMA		MDMA	
2	MDMA	purple	478	MDMA		MDMA	
3	MDMA	pink	490	MDMA		MDMA	
4	MDMA	blue	387	MDMA		MDMA	
5	MDMA	beige	473	MDMA		MDMA	
6	MDMA	orange	435	MDMA		MDMA	
7	MDMA	turquoise	390	MDMA		MDMA	
8	MDMA	pink	508	MDMA		MDMA	
9	MDMA	yellow	422	MDMA		MDMA	
10	MDMA	white	482	MDMA		MDMA	
11	MDMA	purple	461	MDMA		MDMA	
12	MDMA	brown	452	MDMA		MDMA	
13	MDMA	pink	499	MDMA		MDMA	
14	MDMA	orange	445	MDMA		MDMA	
16	MDMA	red	399	MDMA		MDMA	
17	MDMA	white	491	MDMA		MDMA	
18	MDMA	purple	500	MDMA		MDMA	
19	MDMA	yellow	557	MDMA		MDMA	
20	MDMA	grey	385	MDMA		MDMA	
21	MDMA	pink	420	MDMA		MDMA	
22	MDMA	grey	449	MDMA		MDMA	
23	MDMA	pink	481	MDMA		MDMA	
24	MDMA	green	490	MDMA		MDMA	
25	MDMA	blue	260	MDMA		MDMA	

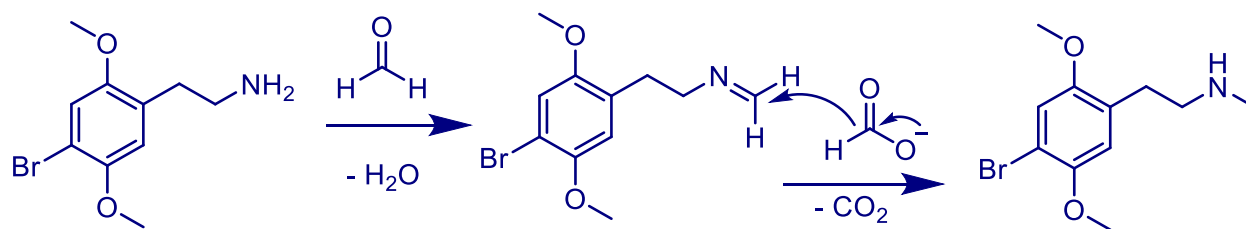
**Table S2.** (part 1 of 3) Results of both electrochemical sensors on the ecstasy tablet set including the obtained electrochemical fingerprint (EF).

TABLET ID	IDENTITY	COLOR	WEIGHT (mg)	MDMA SENSOR OUTPUT	MDMA SENSOR CURVE	MDMA/2C-B SENSOR OUTPUT	MDMA/2C-B SENSOR CURVE
26	MDMA	blue	345	MDMA		MDMA	
27	MDMA	purple-pink	474	MDMA		MDMA	
28	MDMA	pink	490	MDMA		MDMA	
29	MDMA	grey	414	MDMA		MDMA	
30	MDMA	grey	450	MDMA		MDMA	
31	MDMA	pink	509	MDMA		MDMA	
32	MDMA	orange	563	MDMA		MDMA	
33	MDMA	green	382	MDMA		MDMA	
34	MDMA	yellow	483	MDMA		MDMA	
35	MDMA	orange	496	MDMA		MDMA	
36	MDMA	pink	500	MDMA		MDMA	
37	MDMA	green	453	MDMA		MDMA	
38	MDMA	beige	224	MDMA		MDMA	
39	MDMA	green	560	MDMA		MDMA	
40	MDMA	orange	551	MDMA		MDMA	
101	2C-B	green	220	MDMA		2C-B	
102	4-MMC	yellow	315	/		/	
104	2C-B	oker	212	/		2C-B	
105	2C-B	beige	142*	MDMA		2C-B	
106	2-Br-4,5-DMPEA	red	255	/		/	
107	2-Br-4,5-DMPEA	pink	251	/		2C-B	
108	FA	pink	427	/		/	
109	FA	orange	408	/		/	
110	2C-B	green	148	MDMA		MDMA	

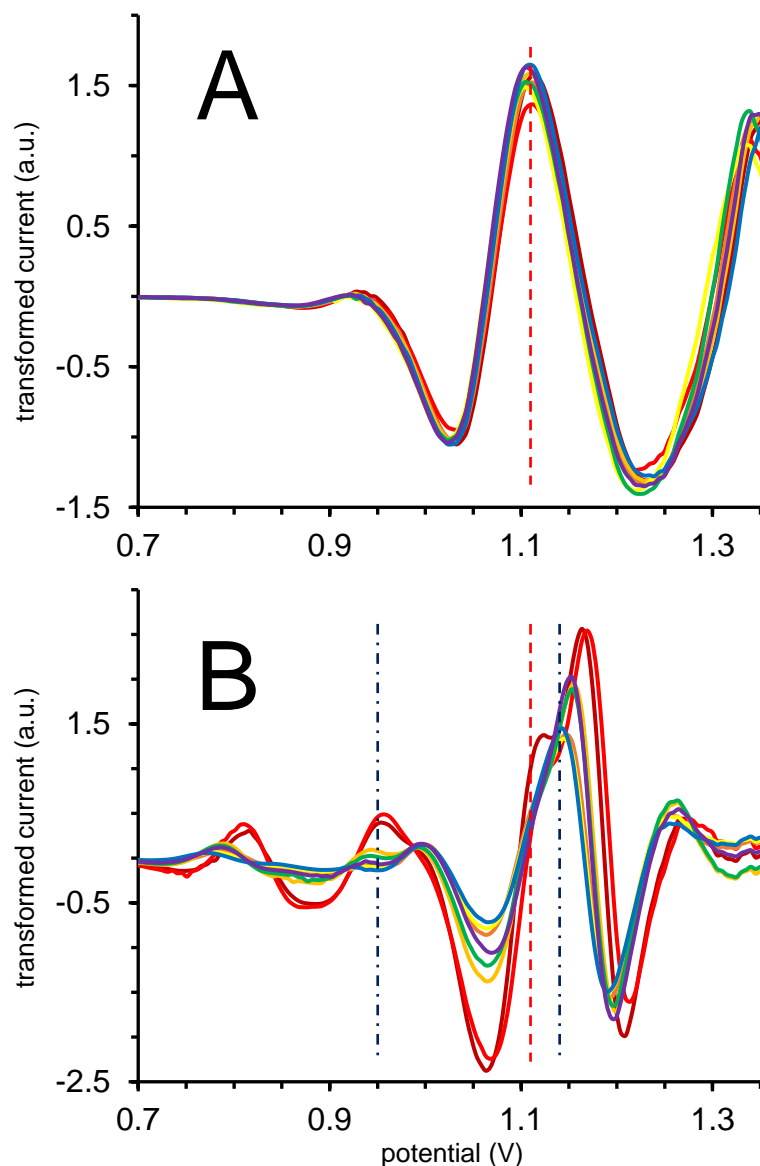
**Table S2.** (part 2 of 3) Results of both electrochemical sensors on the ecstasy tablet set including the obtained electrochemical fingerprint (EF).

TABLET ID	IDENTITY	COLOR	WEIGHT (mg)	MDMA SENSOR OUTPUT	MDMA SENSOR CURVE	MDMA/2C-B SENSOR OUTPUT	MDMA/2C-B SENSOR CURVE
111	2C-B	green	137	MDMA		2C-B	
112	4-FMA	yellow	499	/		/	
113	2-Br-4,5-DMPEA	pink	251	/		2C-B	
114	2C-B	yellow	182	MDMA		2C-B	
115	pentylone	orange	167	/		2C-B	
116	2C-B	green	184	MDMA		2C-B	
117	FMA	green	474	/		/	
118	2C-B	pink	234	MDMA		2C-B	
119	2C-B	green	137	MDMA		2C-B	
120	2C-B	yellow	199	MDMA		2C-B	
121	2C-B	green	134	MDMA		2C-B	
122	2-Br-4,5-DMPEA	red	242	/		/	
123	FA	orange	407	/		/	
124	FA	pink	400	/		/	
125	FMA	brown	541	/		/	
126	4-FA	white	387	/		/	
127	2C-B-fly	pink	183	/		/	
128	FMA	pink	514	/		/	
129	FA	salmon	268	/		/	
130	FMA	blue	269	/		/	
131	mCPP	pink	250	MDMA		/	
132	6-APB	pink	242	/		/	
133	4-FA	pink	294	/		/	

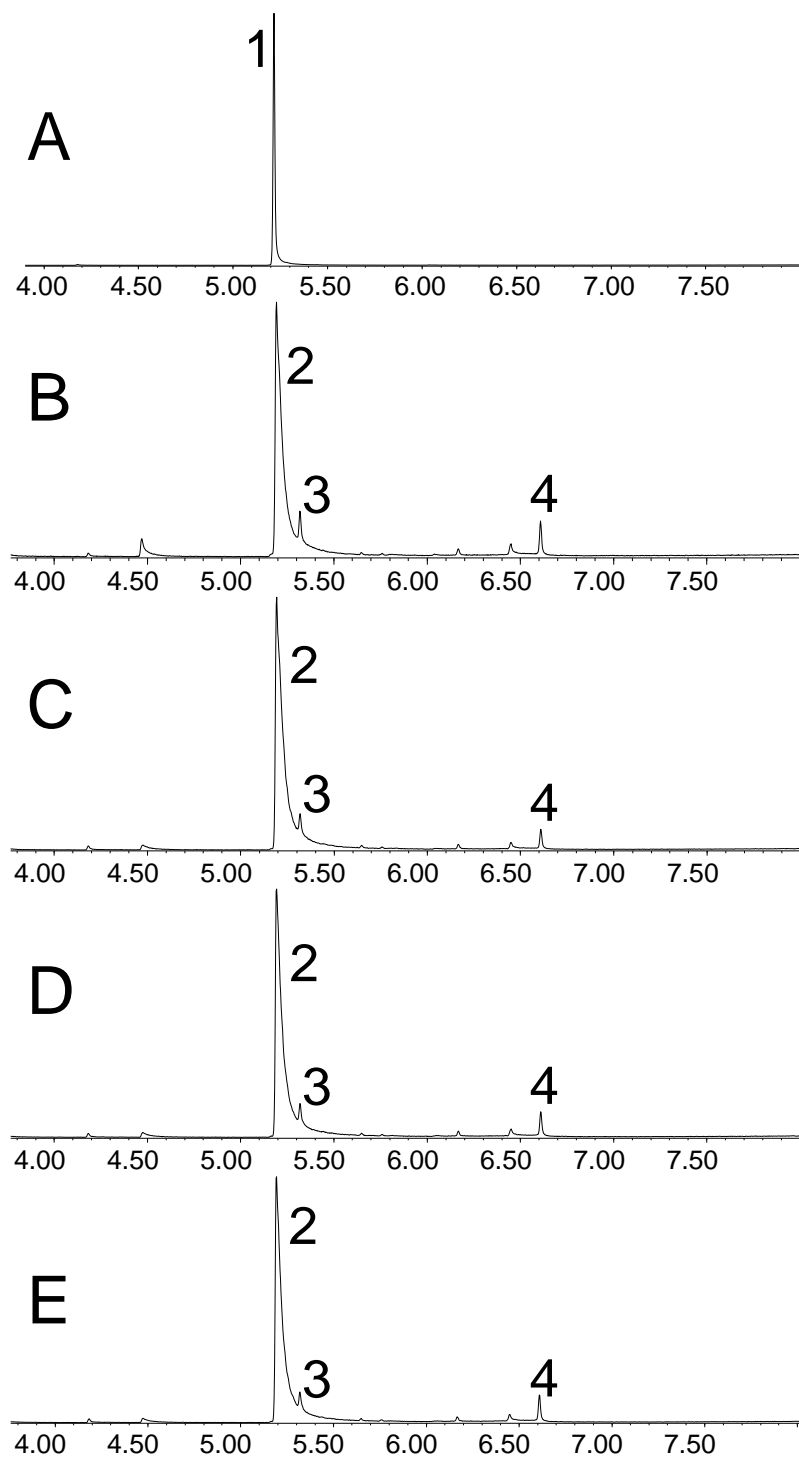
**Table S2.** (part 3 of 3) Results of both electrochemical sensors on the ecstasy tablet set including the obtained electrochemical fingerprint (EF). Tablet 110 was incomplete, indicated with an \* at its weight. Red line indicates the 1.11 V peak diagnostic for MDMA, blue lines indicate the 0.95 V and 1.14 V peaks diagnostic for derivatized 2C-B.



**Figure S2.** Proposed reaction scheme of the *in-situ* derivatization of 2C-B with formaldehyde. Reaction mechanism derived from Schram *et al.*<sup>27</sup>

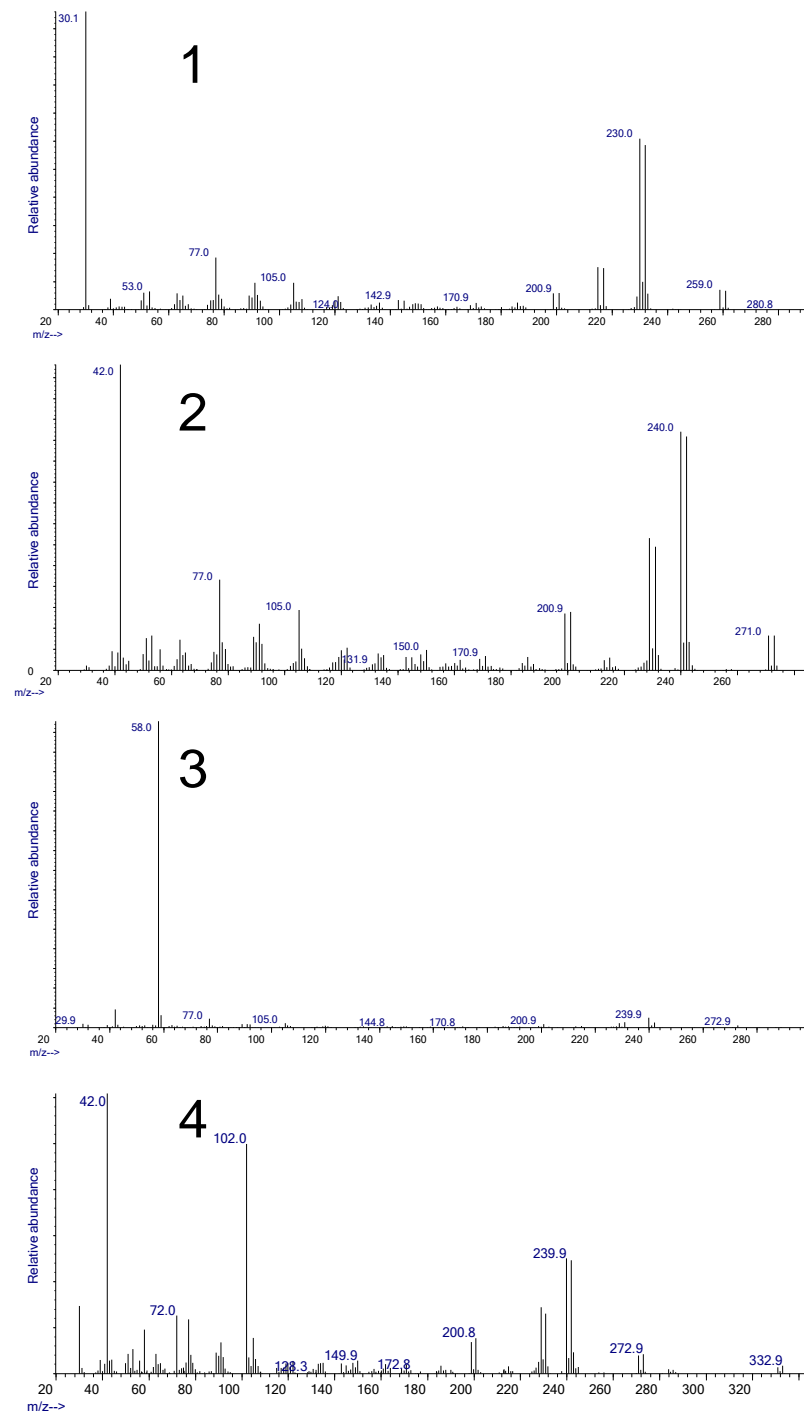


**Figure S3.** Formaldehyde reaction rate plots for MDMA (A) and 2C-B (B). EFs analyzed without waiting time (purple plots), after 20s waiting (blue), 40s (green), 60s (yellow), 90s (orange), 150s (dark orange), 300s (red), 600s (dark red). Red dashed line indicates the 1.11 V peak diagnostic for MDMA, blue dashed lines indicate the 0.95 V and 1.14 V peaks diagnostic for derivatized 2C-B.

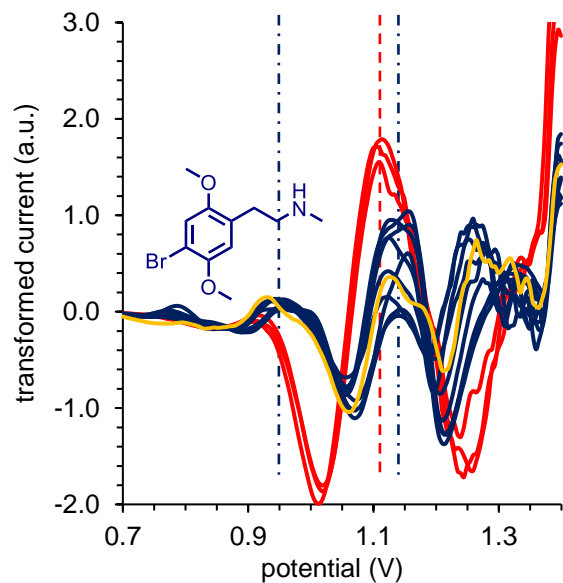


**Figure S4.** Formaldehyde reaction analysis by GC-MS. A: 2C-B sample with no formaldehyde added; B: after 30 sec reaction with formaldehyde; C: 2 min reaction with formaldehyde; D: 10 min reaction with formaldehyde; E: 30 min reaction with formaldehyde. Mass spectra of peaks 1-4 are shown in Figure S4. GC-MS analysis of 1  $\mu$ L dichloromethane from extracts obtained by an alkaline extraction of sample solution with 2 mL dichloromethane.





**Figure S5.** Mass spectra of the GC-MS peaks in Figure S3. 1: 2C-B with  $m/z$  30 base peak originating from the primary amine; 2: methylated 2C-B reaction product with  $m/z$  42 base peak attributed to secondary amine; 3: dimethylated 2C-B with  $m/z$  58 base peak attributed to tertiary amine; 4: secondary methylated 2C-B reaction product.



**Figure S6.** Electrochemical fingerprints (EFs) following two preprocessing steps, *i.e.* a moving average baseline correction and a digital top hat filter transformation. Overlay of 5 MDMA-containing tablets (red) and 10 2C-B-containing tablets (blue) analyzed by the MDMA/2C-B sensor following *in-situ* derivatization with formaldehyde. All identified correctly. Orange plot depict the single 2C-B containing tablet #110 falsely identified as MDMA. Red dashed line indicates the 1.11 V peak diagnostic for MDMA, blue dashed lines indicate the 0.95 V and 1.14 V peaks diagnostic for derivatized 2C-B.