Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Material

Qualitative Analysis of Designer Drugs by Paper Spray Ionisation Mass Spectrometry (PSI-MS)

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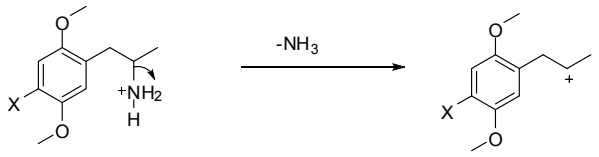
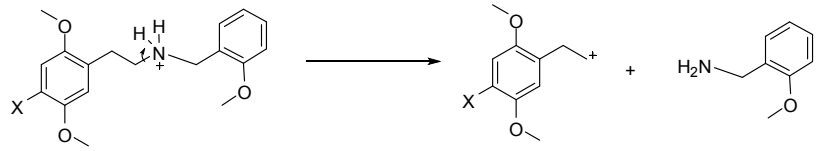
Mechanism I



DOC X = Cl *m/z* 230
DOB X = Br *m/z* 274

X = Cl *m/z* 213
X = Br *m/z* 257

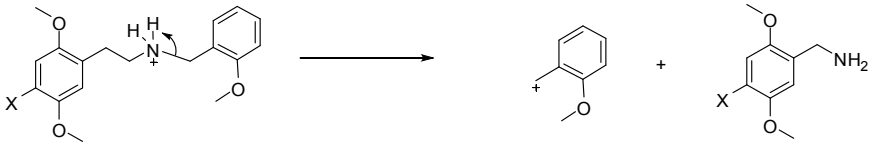
Mechanism II



25C-NBOME X = Cl *m/z* 336
25B-NBOME X = Br *m/z* 380
25I-NBOME X = I *m/z* 428

X = Cl *m/z* 199
X = Br *m/z* 243
X = I *m/z* 291

Mechanism III

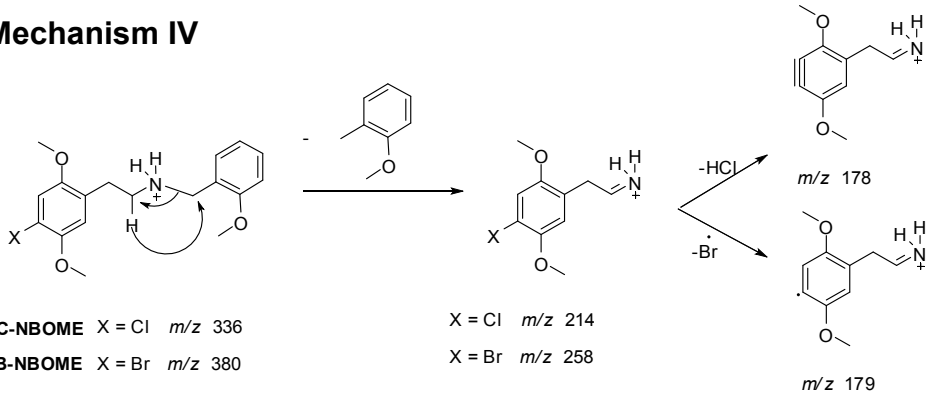


25C-NBOME X = Cl *m/z* 336
25B-NBOME X = Br *m/z* 380
25I-NBOME X = I *m/z* 428

m/z 121

X = Cl
X = Br
X = I

Mechanism IV



25C-NBOME X = Cl *m/z* 336
25B-NBOME X = Br *m/z* 380

X = Cl *m/z* 214
X = Br *m/z* 258

m/z 178

m/z 179

Mechanism V

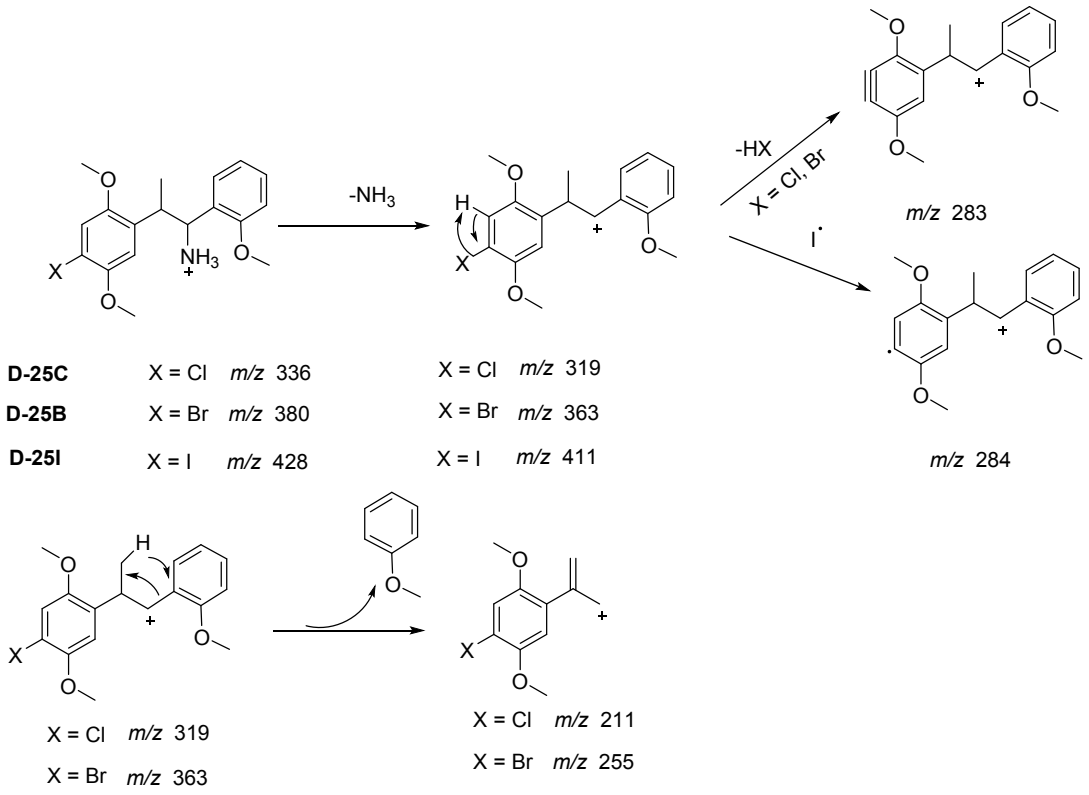


Figure 1S. Fragmentation pathway of six designer drugs analysed by PS(+) MS/MS.

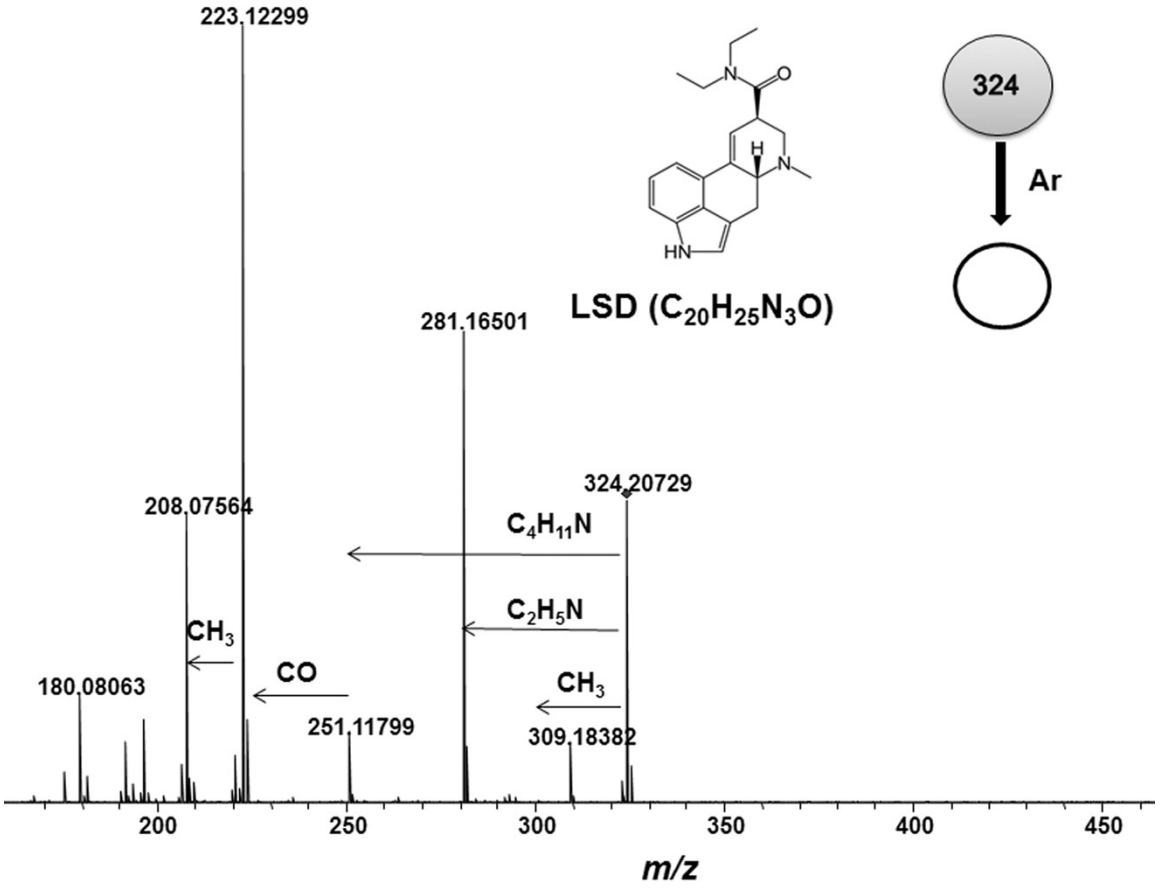


Figure 2S. ESI(+)-MSMS of *m/z* 324 of the LSD sample.

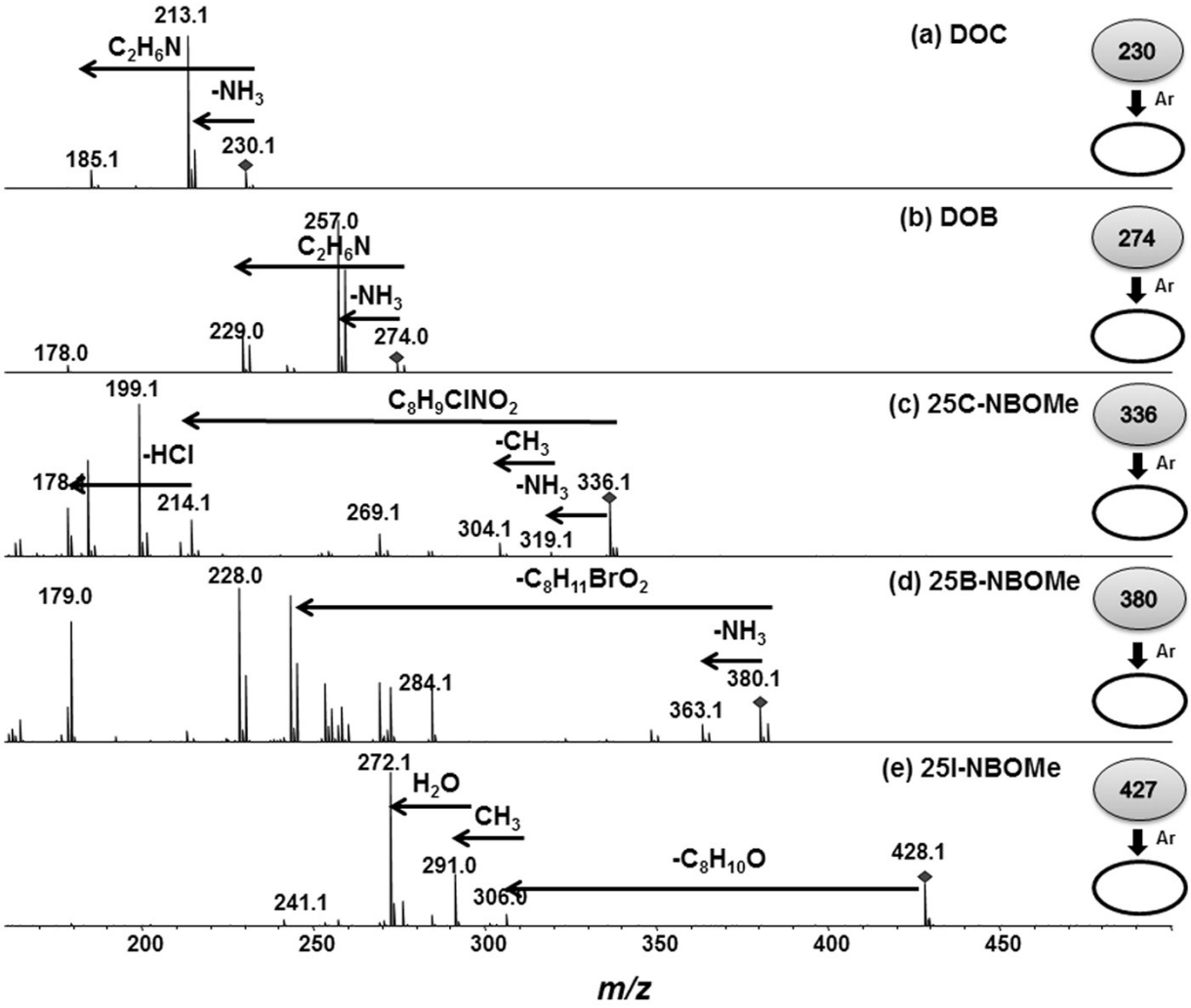


Figure 3S. ESI(+)-MS/MS of the $[M+H]^+$ ions for DOC, DOB, 25C-NBOMe, 25B-NBOME and 25I-NBOMe molecules.

Table 1S. Molecular Formula, DBE, measured and theoretical *m/z* values assignments from the ESI FT-ICR mass spectra data for five designer drugs seized as blotter paper.

Sample	*Formulae [M+H]*$^+$	*m/z* $_{measured}$	*m/z* $_{theoretical}$	DBE	Resolution	Error [ppm]
DOC	$[C_{11}H_{16}ClNO_2 + H]^+$	230.09420	230.09423	4	1700000	0.14
DOB	$[C_{11}H_{16}BrNO_2 + H]^+$	274.04380	274.04372	4	1000000	-0.30
25C-NBOMe	$[C_{18}H_{22}ClNO_3 + H]^+$	336.13619	336.13610	8	1300000	-0.27
25B-NBOMe	$[C_{18}H_{22}BrNO_3 + H]^+$	380.08534	380.08558	8	560000	-0.63
25I-NBOMe	$[C_{18}H_{22}INO_3 + H]^+$	428.07185	428.07171	8	1000000	-0.33