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Supporting Information

Simple Analytical Strategy for Screening Three Synthetic Cathinones (α-PVT, α-PVP, and MDPV) in Oral Fluids

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NMR structural analysis for methylone, MDPV, MDPPP and α-PVT.

Methylone: RMN 1H (400 MHz, DMSO-d6) δ (ppm): 9.69 (1H, brs, NH), 9.17 (1H, brs, NH), 7.69 (1H, dd, J=8.2, 1.5 Hz, H-6′), 7.53 (1H, d, J=1.5 Hz, H-2′), 7.13 (1H, d, J=8.2 Hz, H-5′), 6.19 (2H, s, H-7′), 5.06 (1H, m, H-2), 2.54 (3H, brs, N-CH3), 1.42 (3H, d, J=7.1 Hz, H-3). RMN 13C (100 MHz, DMSO-d6) δ (ppm): 194.38 (C=O, C-1), 152.77 (Cq, C-4′), 148.26 (Cq, C-3′), 127.41 (Cq, C-1′), 125.88 (CH, C-6′), 108.60 (CH, C-5′), 107.94 (CH, C-2′), 102.53 (O-CH2-O, C-7′), 57.98 (CH, C-2), 30.67 (N-CH3), 15.79 (CH3, C-3).

MDPV: RMN 1H (400 MHz, DMSO-d6) δ (ppm): 10.26 (1H, brs, NH), 7.77 (1H, dd, J=8.2, 1.4 Hz, H-6′), 7.57 (1H, d, J=1.4 Hz, H-2′), 7.16 (1H, d, J=8.2 Hz, H-5′), 6.20 (2H, s, H-7′), 5.45 (1H, m, H-2), 3.60/3.22 and 3.44/2.99 (4H, m, H¬ 1′′/H-4′′, N-CH2), 2.12-1.80 (4H, m, H-2′′/H-3′′), 1.90 (2H, m, H 3), 1.11 (2H, m, H-4), 0.79 (3H, t, J=7.2 Hz, H-5). RMN 13C (100 MHz, DMSO-d6) δ (ppm): 194.55 (C=O, C-1), 153.20 (Cq, C 4′), 148.38 (Cq, C-3′), 128.97 (Cq, C-1′), 126.25 (CH, C-6′), 108.65 (CH, C-5′), 107.86 (CH, C-2′), 102.69 (O-CH2-O, C-7′), 67.16 (CH, C-2), 53.82 and 51.90 (N-CH2, C-1′′/C 4′′), 32.09 (CH2, C-3), 22.83 (CH2, C 2′′/C-3′′), 17.36 (CH2, C-4), 13.74 (CH3, C-5).

MDPPP: RMN 1H (400 MHz, DMSO-d6) δ (ppm): 10.69 (1H, brs, NH), 7.70 (1H, brd, J=8.0 Hz, H-6′), 7.53 (1H, brs, H-2′), 7.14 (1H, d, J=8.0 Hz, H-5′), 6.19 (2H, s, H-7′), 5.41 (1H, m, H-1), 3.60/3.18 and 3.49/3.01 (4H, m, H-1′′/H-4′′, N-CH2), 2.11-1.81 (4H, m, H-2′′/H-3′′), 1.48 (3H, d, J=6.8 Hz, H-3). RMN 13C (100 MHz, DMSO-d6) δ (ppm): 194.37 (C=O, C-1), 152.95 (Cq, C-4′), 148.30 (Cq, C-3′), 126.05 (CH, C-6′), 108.65 (CH, C-5′), 108.00 (CH, C-2′),102.60 (O-CH2-O, C-7′), 63.83 (CH, C-1), 53.04 and 51.81 (N-CH2, C 1′′/C-4′′*), 23.10 (CH2, C-2′′/C-3′′), 16.16 (CH3, C-3).

α-PVT: RMN 1H (400 MHz, DMSO-d6) δ (ppm): 10.74 (1H, brs, NH), 8.32 (1H, d, J=3.2 Hz, H-2′), 8.27 (1H, d, J=4.4 Hz, H-4′), 7.37 (1H, dd, J=4.4, 3.2 Hz, H-3′), 5.40 (1H, m, H-2), 3.62/3.23 and 3.42/3.06 (4H, m, H-1′′/H-4′′), 1.95 (2H, m, H-3), 2.06-1.85 (4H, m, H-2′′/H-3′′), 1.18 (2H, m, H-4), 0.83 (3H, t, J=7.3 Hz, H-5). RMN 13C (100 MHz, DMSO-d6) δ (ppm): 189.02 (C=O, C-1), 141.73 (Cq, C-1′), 138.69 (CH, C-4′), 136.61 (CH, C-2′), 129.58 (CH, C-3′), 67.14 (CH, C-2), 53.10 and 52.02 (N-CH2, C 1′′/C-4′′), 32.17 (CH2, C-3), 22.82 (CH2, C-2′′/C-3′′), 17.89 (CH2, C-4), 13.72 (CH3, C-5).

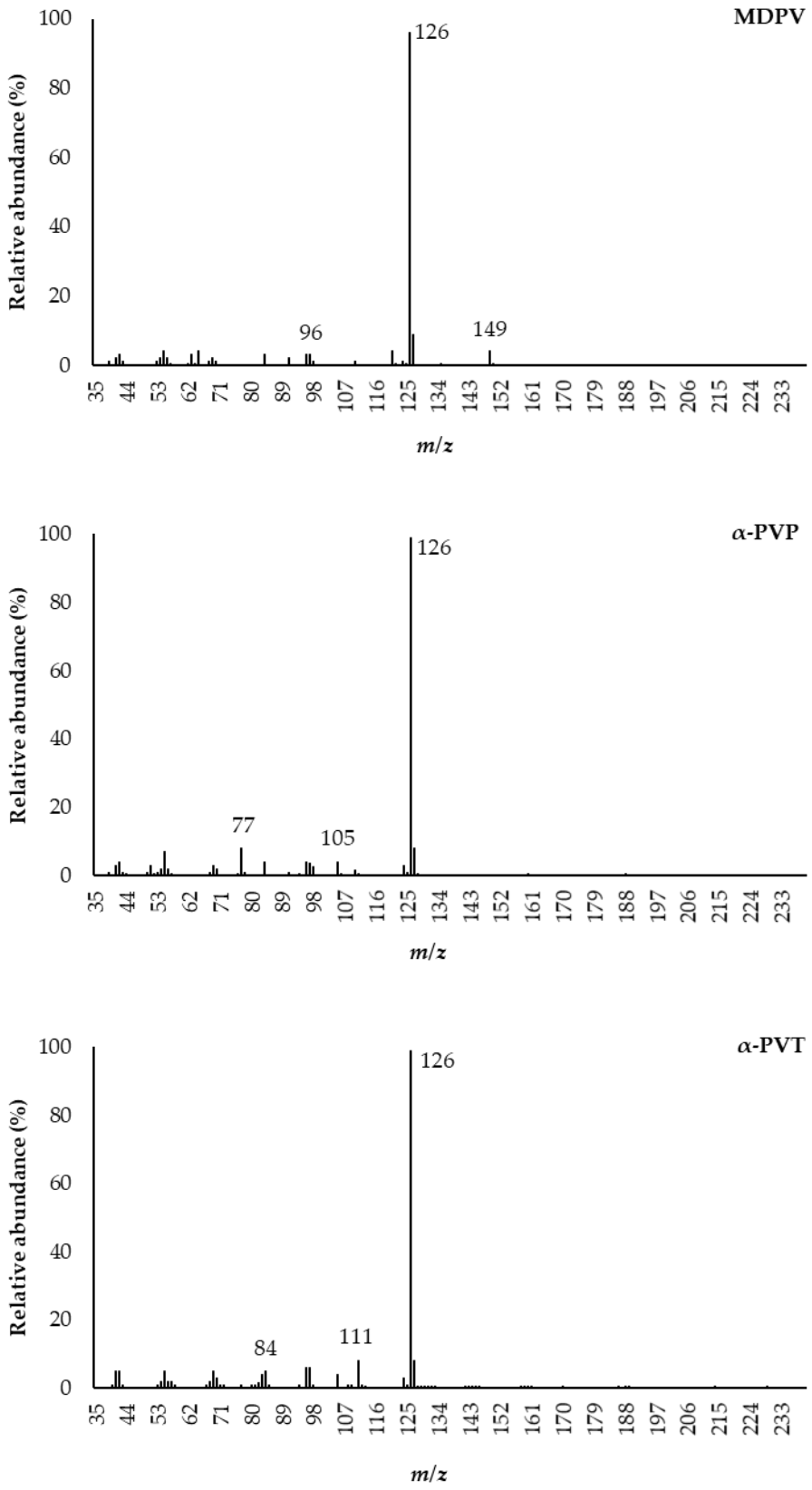

Figure S1. Mass spectra of α-PVP, α-PVT and MDPV obtained by GC-MS under full-scan mode.

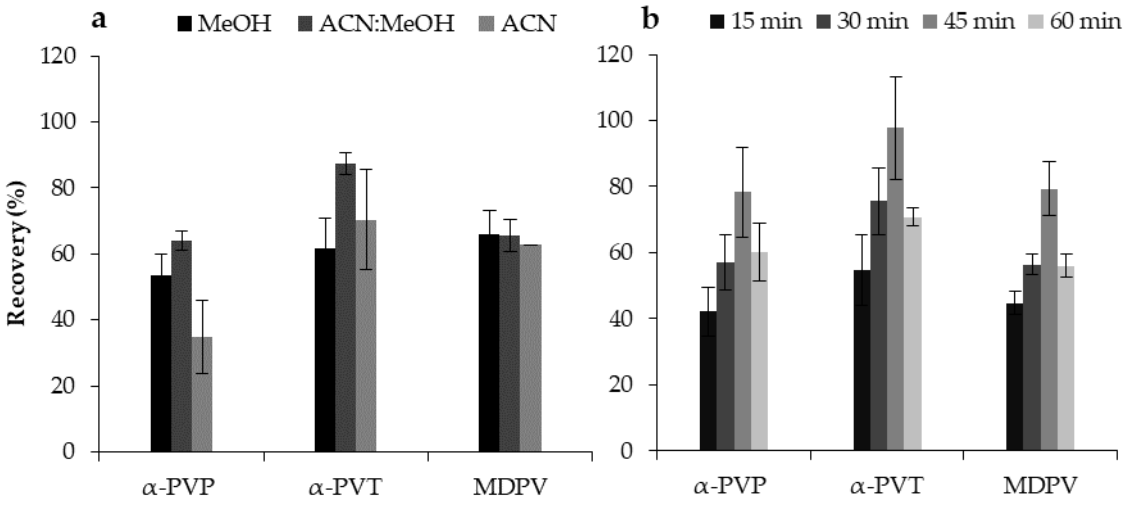

Figure S2. Effect of the back-extraction solvent (a) time (b) on the microextraction of the three SCs in aqueous media, obtained by BAμE-μLD/GC-MS(SIM). The error bars represent the standard deviation of three replicates.

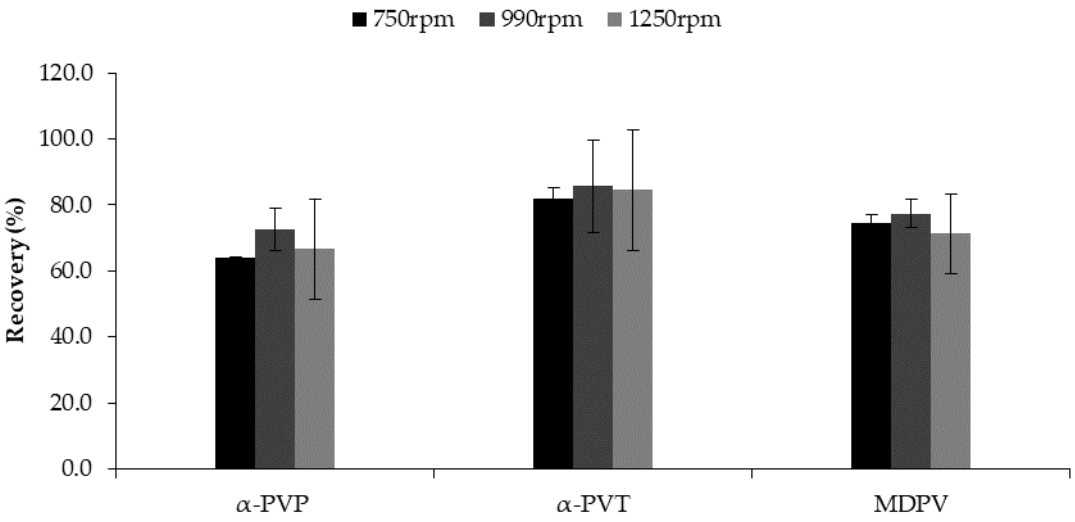

Figure S3. Effect of stirring rate on the microextraction of the three SCs in aqueous media, obtained by BAμE-μLD/GC-MS(SIM). The error bars represent the standard deviation of three replicates.

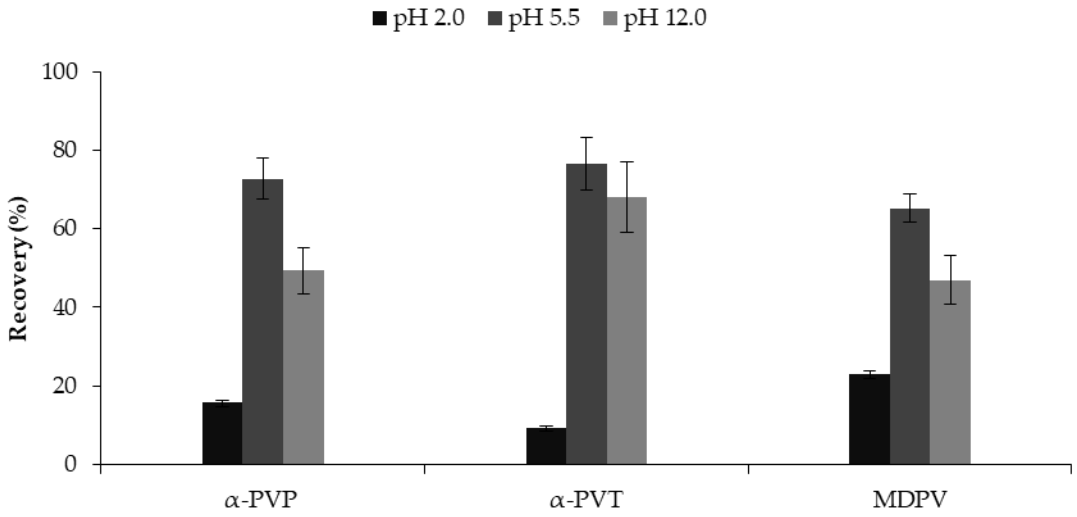

Figure S4. Effect matrix pH on the microextraction of the three SCs in aqueous media, obtained by BAμE-μLD/GC-MS(SIM). The error bars represent the standard deviation of three replicates.

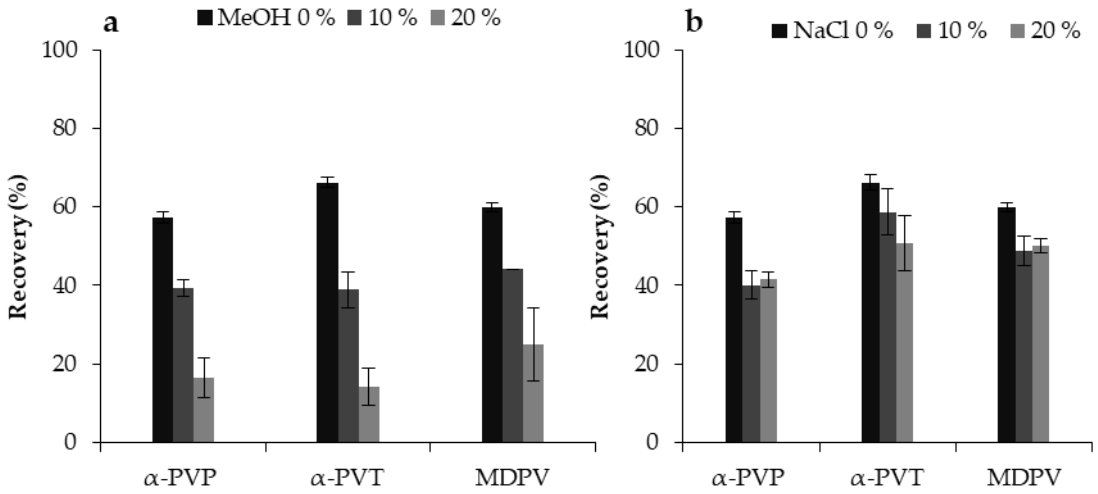

Figure S5. Effect of matrix MeOH (a) and NaCl (b) content on the microextraction of the three SCs in aqueous media, obtained by BAμE-μLD/GC-MS(SIM). The error bars represent the standard deviation of three replicates.