

Supplementary Material

Sensitive detection of synthetic cannabinoids in human blood using magnetic polydopamine molecular imprinted polymer nanocomposites

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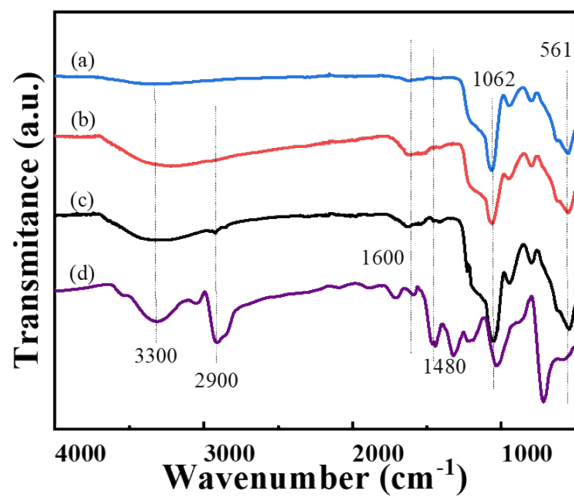


Figure S1. FT-IR spectra of (a) Fe₃O₄@SiO₂ NPs (b) PDA@Fe₃O₄ NIP, (c) PDA@Fe₃O₄ MIP with 9CH embedded and (d) 9CH.

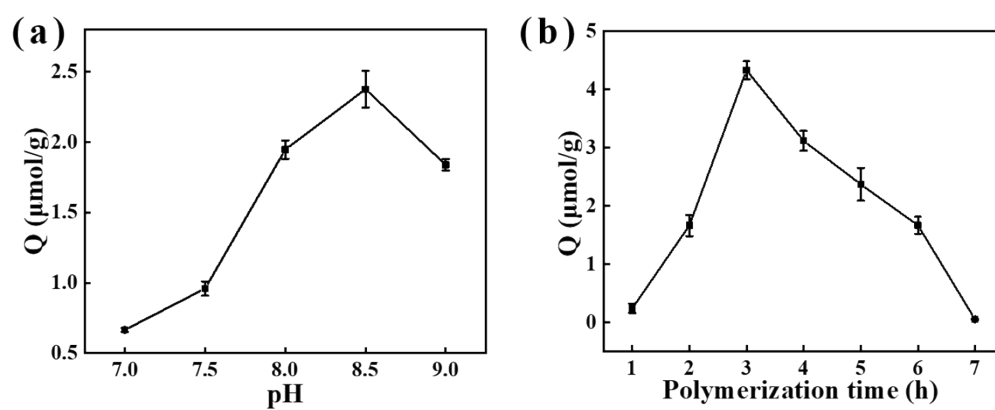


Figure S2. Optimization of (a) pH and (b) polymerization time for the synthesis of PDA@Fe₃O₄ MIP

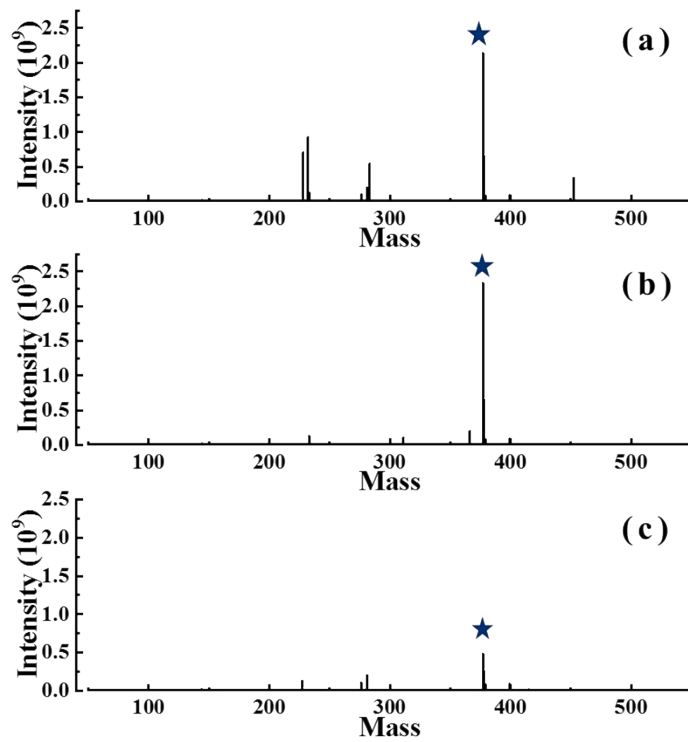


Figure S3. Mass spectrometry is used to analyze the content of 5F-PB-22 in human blood. (a) without MIP pretreatment, (b) extracted by PDA@Fe₃O₄ MIP, and(c) extracted by PDA@Fe₃O₄ NIP.

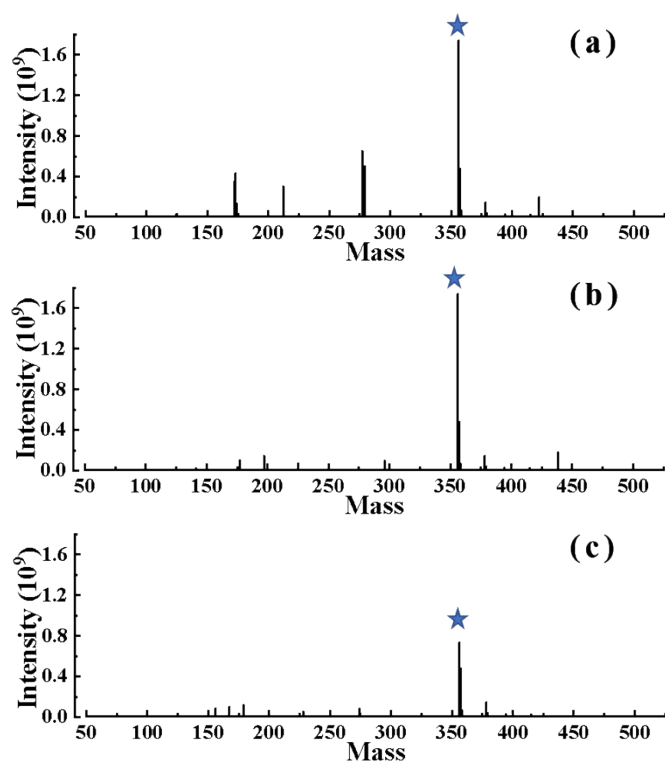


Figure S4. Mass spectrometry is used to analyze the content of JWH-122 in human blood. (a) without MIP pretreatment, (b) extracted by PDA@Fe₃O₄ MIP, and(c) extracted by PDA@Fe₃O₄ NIP.

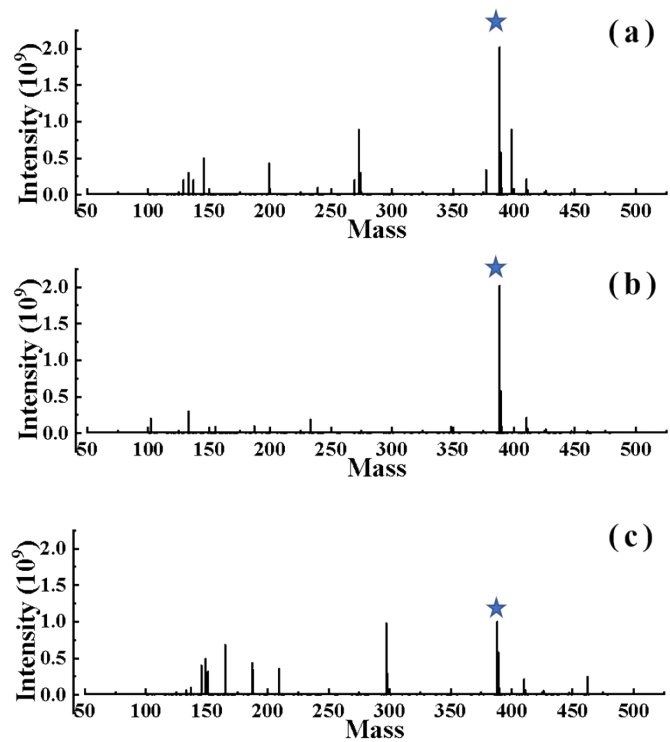


Figure S5. Mass spectrometry is used to analyze the content of EAM-2201 in human blood. (a) without MIP pretreatment, (b) extracted by PDA@Fe₃O₄ MIP, and (c) extracted by PDA@Fe₃O₄ NIP.

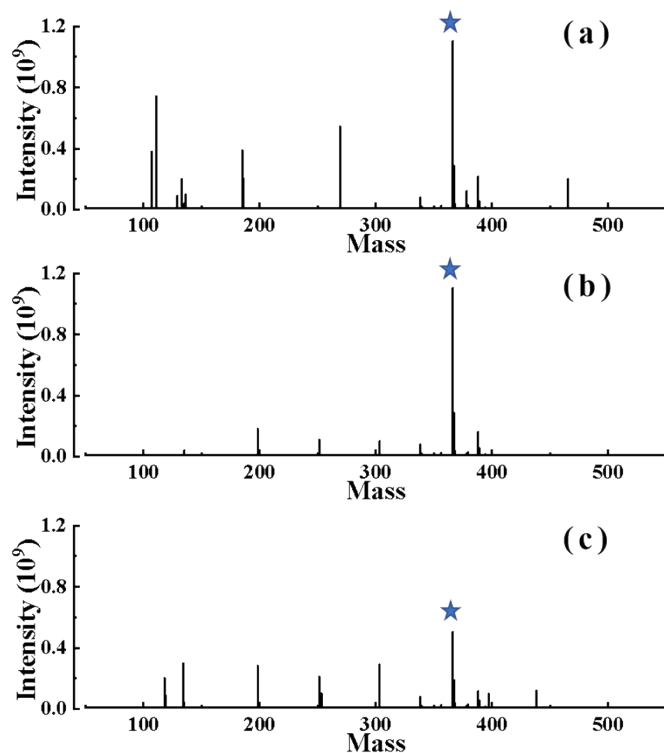


Figure S6. Mass spectrometry is used to analyze the content of APINACA in human blood. (a) without MIP pretreatment, (b) extracted by PDA@Fe₃O₄ MIP, and (c) extracted by PDA@Fe₃O₄ NIP.

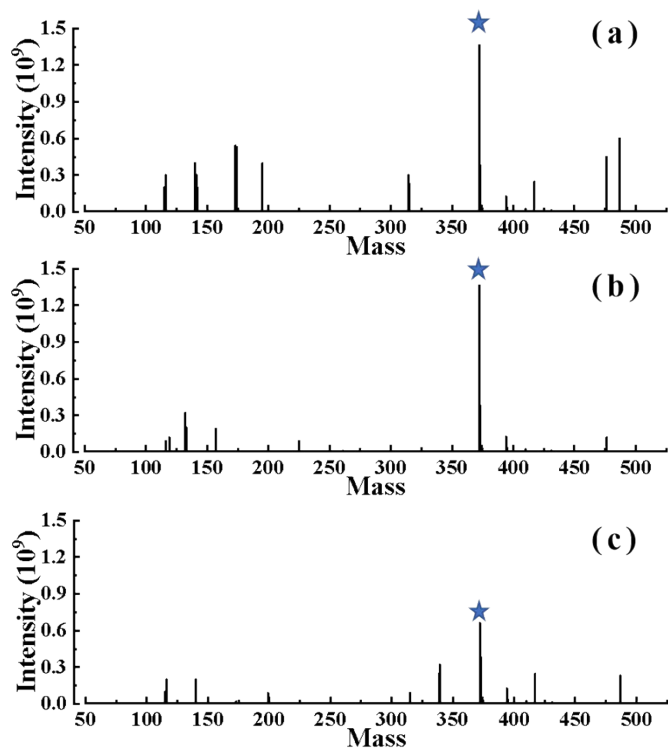


Figure S7. Mass spectrometry is used to analyze the content of JWH-081 in human blood. (a) without MIP pretreatment, (b) extracted by PDA@Fe₃O₄ MIP, and (c) extracted by PDA@Fe₃O₄ NIP.

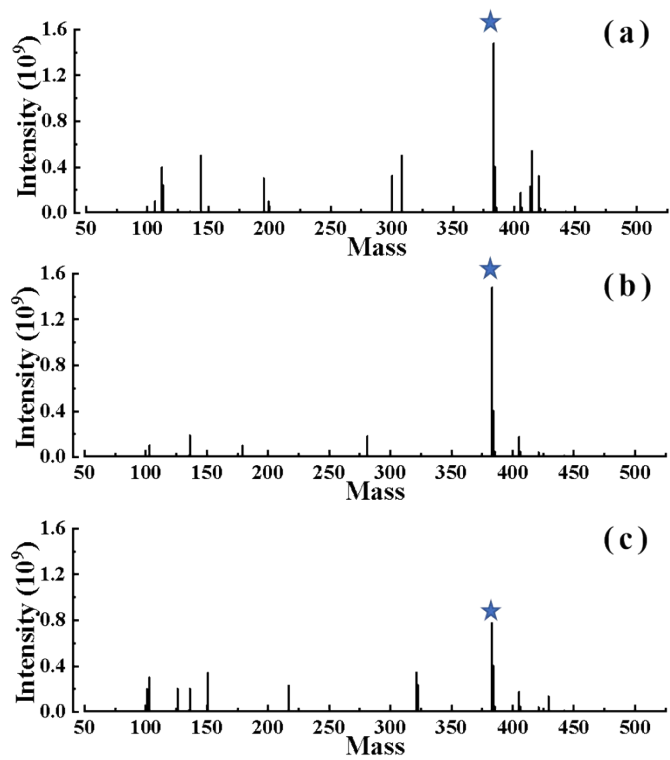


Figure S8. Mass spectrometry is used to analyze the content of STS-135 in human blood. (a) without MIP pretreatment, (b) extracted by PDA@Fe₃O₄ MIP, and (c) extracted by PDA@Fe₃O₄ NIP.

Table S1: Conditions for liquid chromatography

| HPLC parameters | |
|-----------------------|---|
| Columns | Agilent Eclipse plus C18 (3 x 100 mm x 2.1 μ m) |
| Eluent | A: Methanol B: 5 mmol Ammonium formate / 0.1% Methanoic acid |
| Injection Volume | 10 μ L |
| Flow Rate | 500 μ L/mL |
| Column temperature | 40 $^{\circ}$ C |

Table S2: Conditions for mass spectrometry

| MS parameters | |
|--|-------------------------|
| Polarity | Positive |
| Ionization source | Electrospray Ionization |
| Sweep gas flow rate | 2 arb |
| Spray voltage | 3.5 kV |
| Sheath gas flow rate | 45 arb |
| Aux gas flow rate | 10 arb |
| Aux gas heater temp | 400 °C |
| Capillary temp | 320 °C |
| Resolution | 70000 |
| Automatic gain control (AGC) target | 2e6 |
| Collision energy (CE) | 40 eV |
| Scan range | 50 to 400 m/z |
| Maximum IT | 100 ms |

Table S3. Mass spectrometric characterization parameters of six synthetic cannabinoids

| Compounds | RT (min) | Precursor ion [M+H] ⁺ (m/z) | Fragmentation ions (m/z) |
|-----------|-------------|---|-----------------------------|
| JWH-122 | 10.37 | 356.2010 | 214.1227, 169.0649 |
| JWH-081 | 9.82 | 372.1954 | 214.1227, 185.0597 |
| EAM2201 | 5.70 | 388.2069 | 232.1130, 183.0804 |
| 5F-PB-22 | 8.15 | 377.1662 | 232.1133, 144.0444 |
| STS-135 | 15.26 | 383.2486 | 232.1133, 135.1169 |
| APINACA | 8.34 | 366.2540 | 135.1168, 107.0855 |

Table S4. Optimization of the ratio of Fe₃O₄, DA and 9CH

| Entry | Fe ₃ O ₄ (mg) | DA (mg) | 9CH (mg) | Q ($\mu\text{mol}\cdot\text{g}^{-1}$) |
|-------|--|------------|-------------|--|
| 1 | 10 | 5 | 10 | 4.33 |
| 2 | 10 | 7 | 10 | 5.74 |
| 3 | 10 | 10 | 10 | 4.12 |
| 4 | 10 | 15 | 10 | 5.34 |
| 5 | 10 | 7 | 10 | 4.21 |
| 6 | 10 | 7 | 20 | 5.55 |
| 7 | 10 | 7 | 30 | 6.26 |
| 8 | 10 | 7 | 40 | 6.07 |

Other synthesis conditions: polymerization time = 3 h, polymerization of Tris Buffer (10 mL, pH = 8.5) solution.

The concentration of each SC is 1 $\mu\text{g}/\text{mL}$ for the adsorption capacity evaluation.