Real-Time, Real-World, Real Small: Unlocking Molecular Secrets with Mass Spectrometry

Single Particle Mass Spectrometry: Revealing the Hidden Chemistry of Every Particle

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Aerosols and airborne particulates (ranging from nm to μm in size) originate from both natural and anthropogenic sources and have profound impacts on *health*, the *environment*, *climate*, and *security*. This cutting-edge research platform enables real-time analysis of particle size, composition, and mixing state, while simultaneously detecting metals (cations and anions) and organic molecules at single-particle resolution. SPMS application supports early aerosol hazard warnings (*Figures 1–3*).

Figure 1. Workflow of the detection technology in the HazarDust project [1]. Core is the single-particle mass spectrometer with tailored laser ionisation schemes.
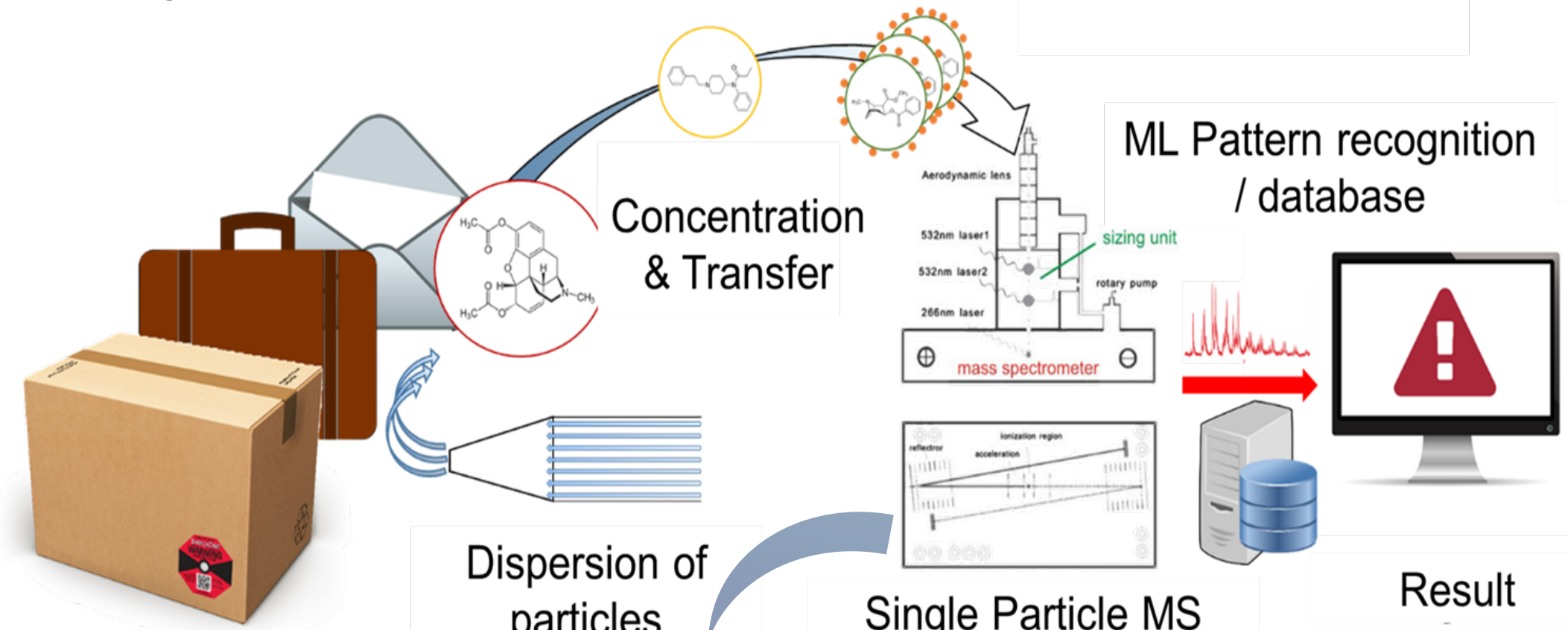
Figure 2. Schematic view of the single-particle detection of bipolar time of flight mass analyser. **(a)** The particle is hit by an IR laser pulse for desorption of organics. **(b)** After 14 μs, the expanding plume (red) is illuminated with a broad UV laser beam (blue) for Resonance-enhanced multiphoton ionisation (REMPI). The same pulse is reflected and focused on the particle residue (black), ionising refractory inorganics via Laser Desorption Ionisation (LDI) with much higher intensity. [2].
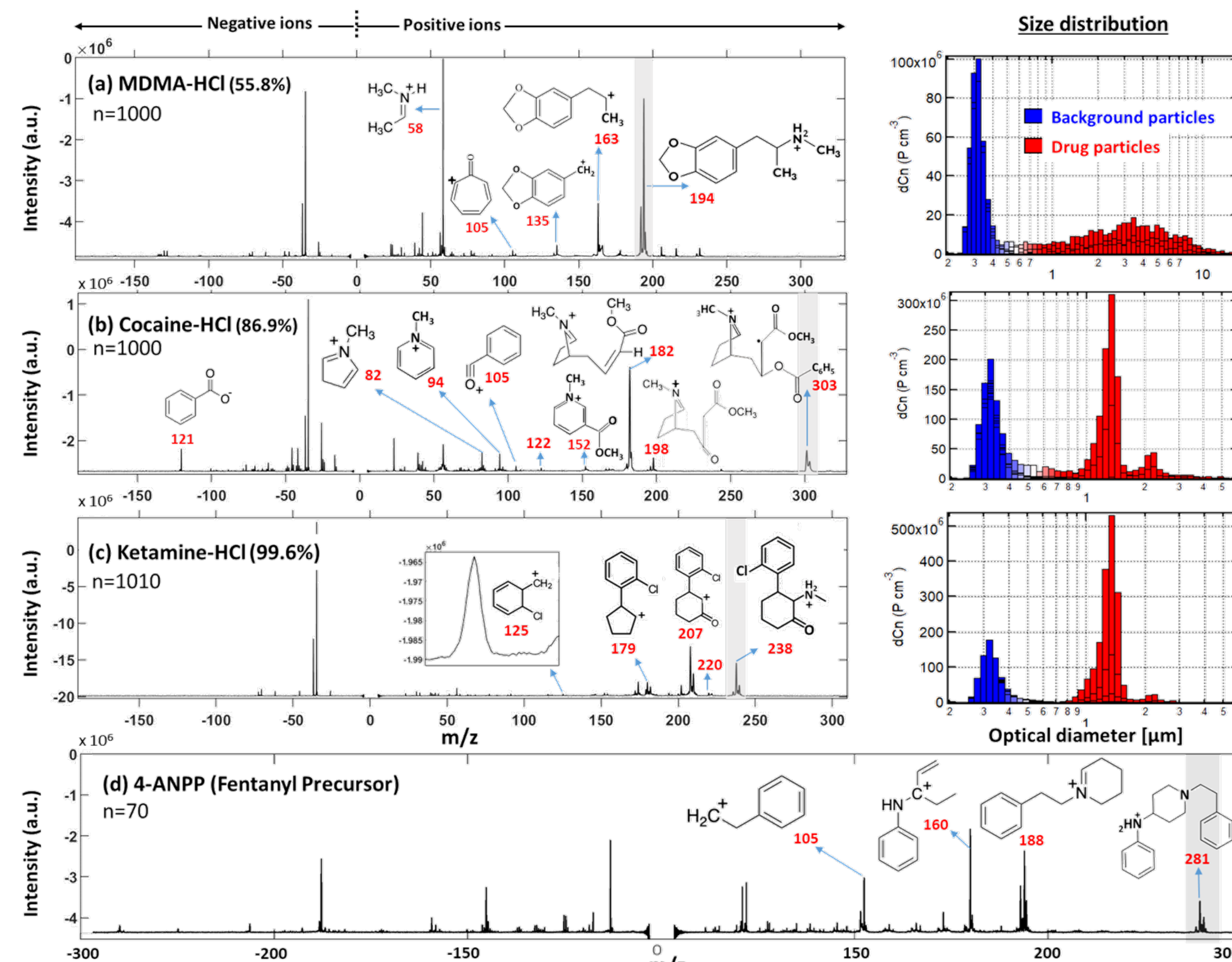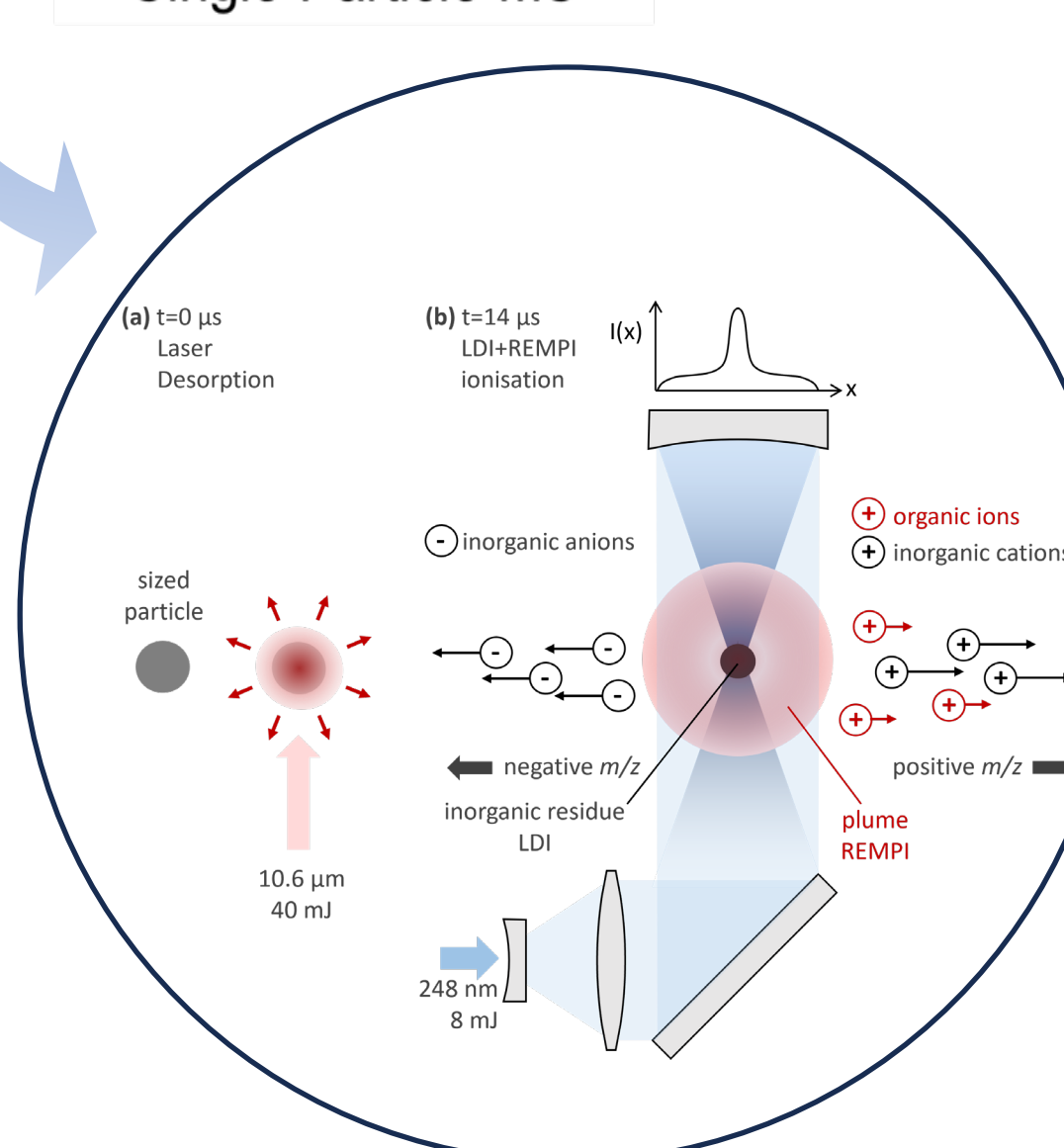
Figure 3. Narcotics were provided by the Forensic Science Institute, Bavarian State Criminal Police Office. At an ionisation laser wavelength of 248 nm (resonant with aromatic ring structures), all substances showed a molecule ion peak (marked in gray) as well as characteristic fragments for the majority of particles [3]. This also applies to 4-anilino-N-phenethylpiperidine (4-ANPP), a structurally related precursor of fentanyl - the key substance in the U.S. opioid crisis.

Smart Surfaces, Rapid Detection: Ambient Mass Spectrometry for Ultra-Trace Detection

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Our SMART Ambient Mass Spectrometry (AMS) platform enables *in-situ* analysis for the rapid detection of trace levels of emerging and socially relevant substances (*Figure 4*).

Unlike conventional methods that rely on lengthy and costly chromatographic techniques, AMS offers direct analysis. However, complex sample matrices can lead to ion suppression, compromising the reliability of trace detection.
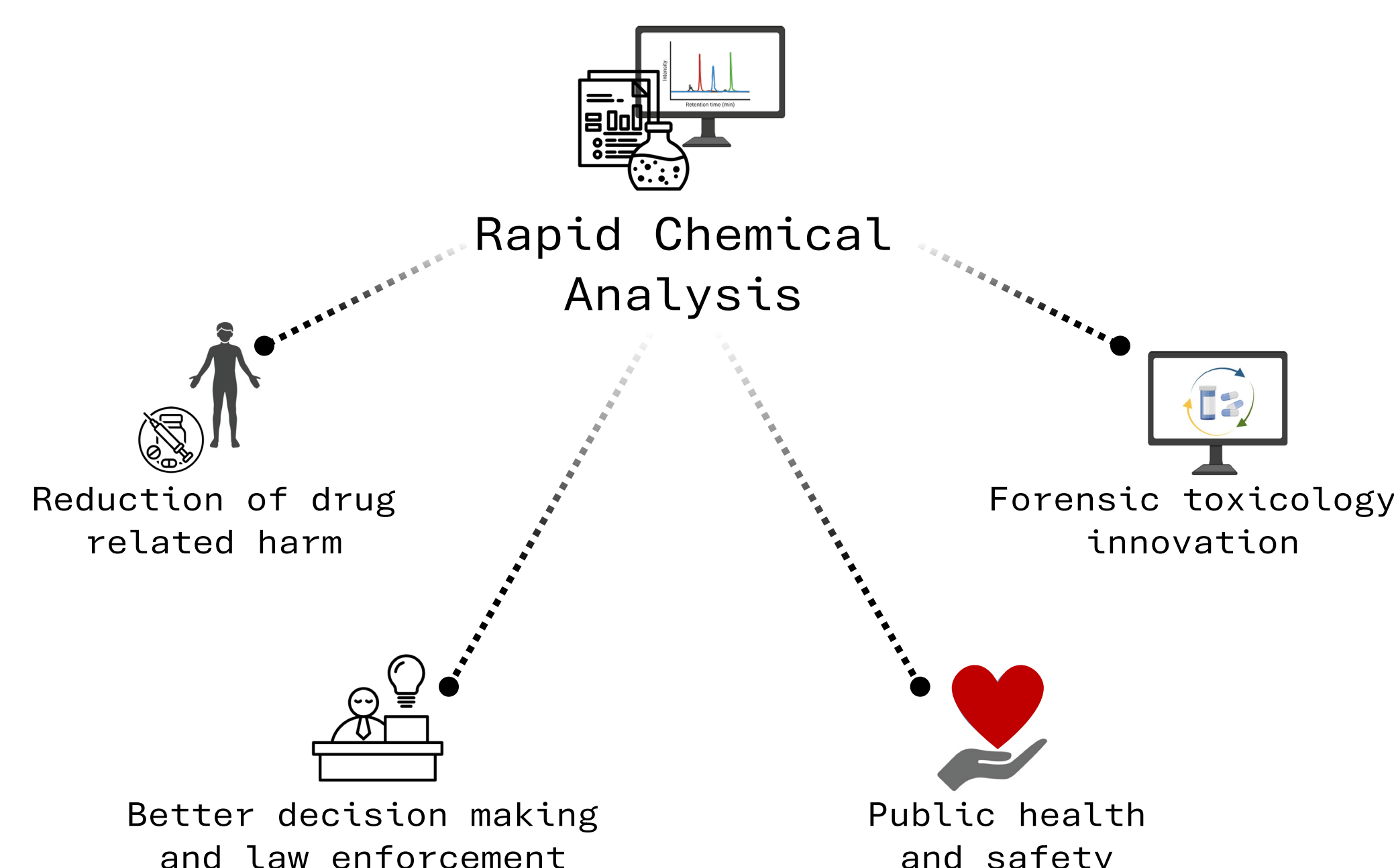

Figure 4. Societal impacts of rapid detection techniques on drug testing. Image created in https://BioRender.com using icons from Noun Project.

To overcome this challenge, smart materials are being developed to interface with AMS, selectively capturing target molecules and thereby enhancing analytical performance[4-9] (*Figure 5*).
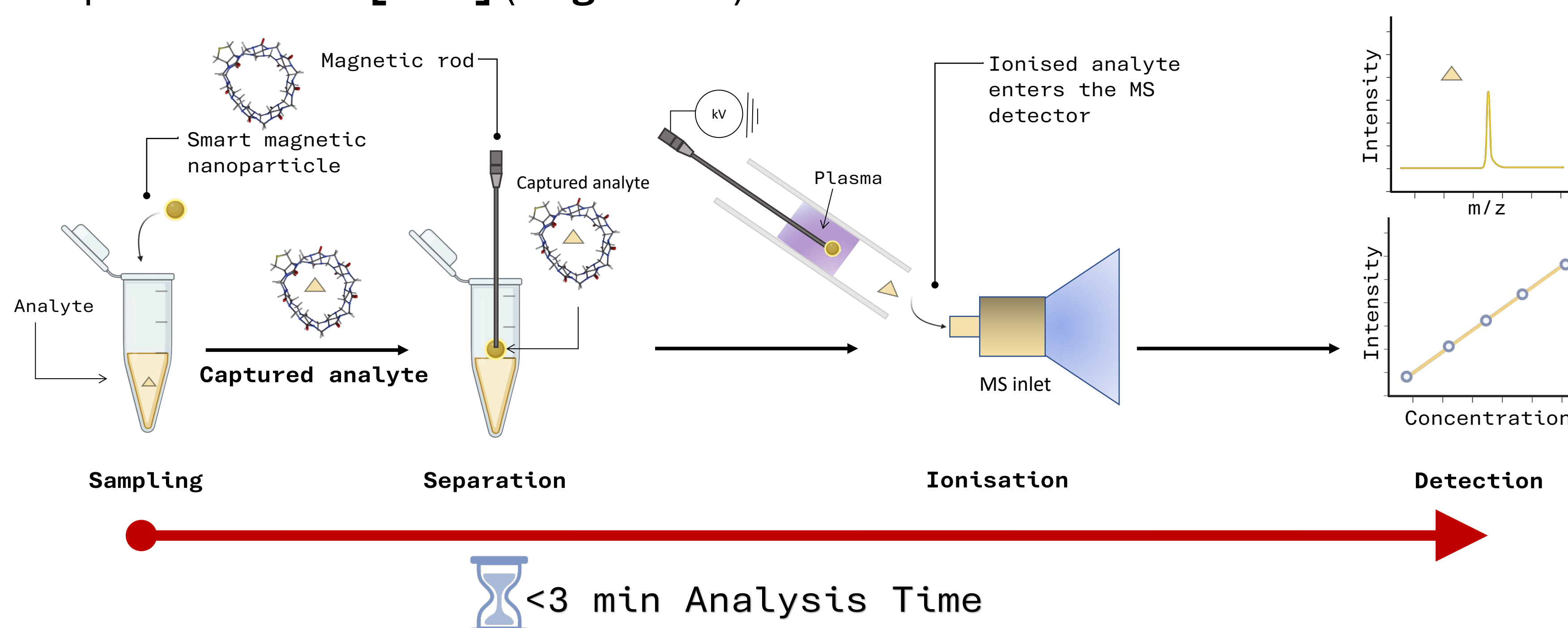

⏳ **<3 min Analysis Time**

Figure 5. Our one-step enrichment technique uses functionalised materials to selectively capture target molecules from complex sample matrices. This approach mitigates ion suppression, significantly reduces instrument time, and enhances method sensitivity. Image was created using icons from https://BioRender.com .

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Target Collaborators

• Forensics • Environmental monitoring • Manufacturing & industry • Health & medicine • Food safety •

References

[1] Passig, J.; Zimmermann, R., **2021**; Wiley-VCH, pp 359.

[2] Schade, J.; Passig, J.; Irsig, R., *et al.*, Anal. Chem. **2019**, 91 (15), 10282.

[3] Hakkim, H., Hehet, M., Schmidt, M., **Dumlao, M.**, *et al.*, **2025**, under preparation.

[4] Zhou, Y; Ai, J.; Ye, Z., *et al.*, Adv. Sci. **2025**, e02721.

[5] **Dumlao, M.C.**; Jiang, L.; *et al.*, Mol. **2024**, 29, (24), 6053.

[6] Zhang, J.; Teng, F., *et al.*, Adv. Mat **2024**, 36 (18), 2311431.

[7] Millán-Santiago, J.; Lucena, R.; Cárdenas, S. J. Sep. Sci. **2022**, 45 (1), 223-232.

[8] Abdulrahman, A.; Hamoud, M.M.; Mandadapu, V.; Zhao, Y.; Chen, M.; **Day, A.I.**, Eur.J. Org. Chem.,**2025**, 28, (14), e202401425.

[9] Bade, R.; Nadarajan, D.; *et.al.*, Addict. **2025**, 120, 1739–1746.