



MEDIZINISCHE
UNIVERSITÄT WIEN



Suchthilfe
Wien

Für die
Stadt Wien

Direkte Massenspektrometrie zur Analyse psychoaktiver Substanzen

Mag. pharm. Anton Luf

Projektleiter checkit! MUW

Klinisches Institut für Labormedizin

Medizinische Universität Wien

10.03.2026



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checkit! Ist eine wissenschaftliche Kooperation von:



finanziert von:

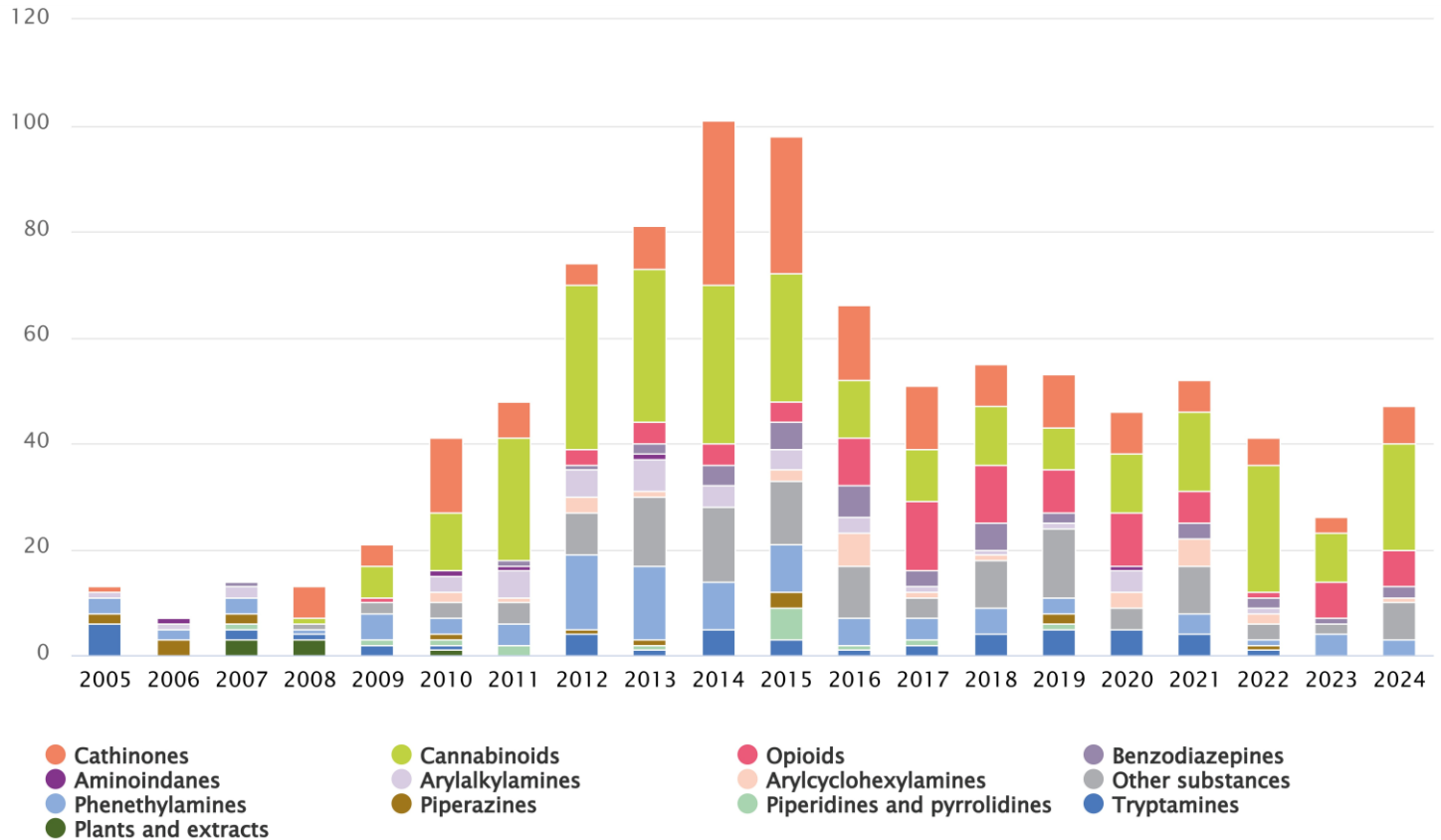


Herausforderungen

- Sehr große und trotzdem zunehmende Anzahl verschiedener neuer psychoaktiver Substanzen (NPS) auf dem Markt
- Hohe Komplexität der Proben (Vielstoffgemische)
- Hohe Variabilität der enthaltenen Dosis
- Auftreten hochpotenter Substanzen
- Verfügbarkeit von Referenzmaterial begrenzt

Neue Psychoaktive Substanzen – Aktuelle Situation

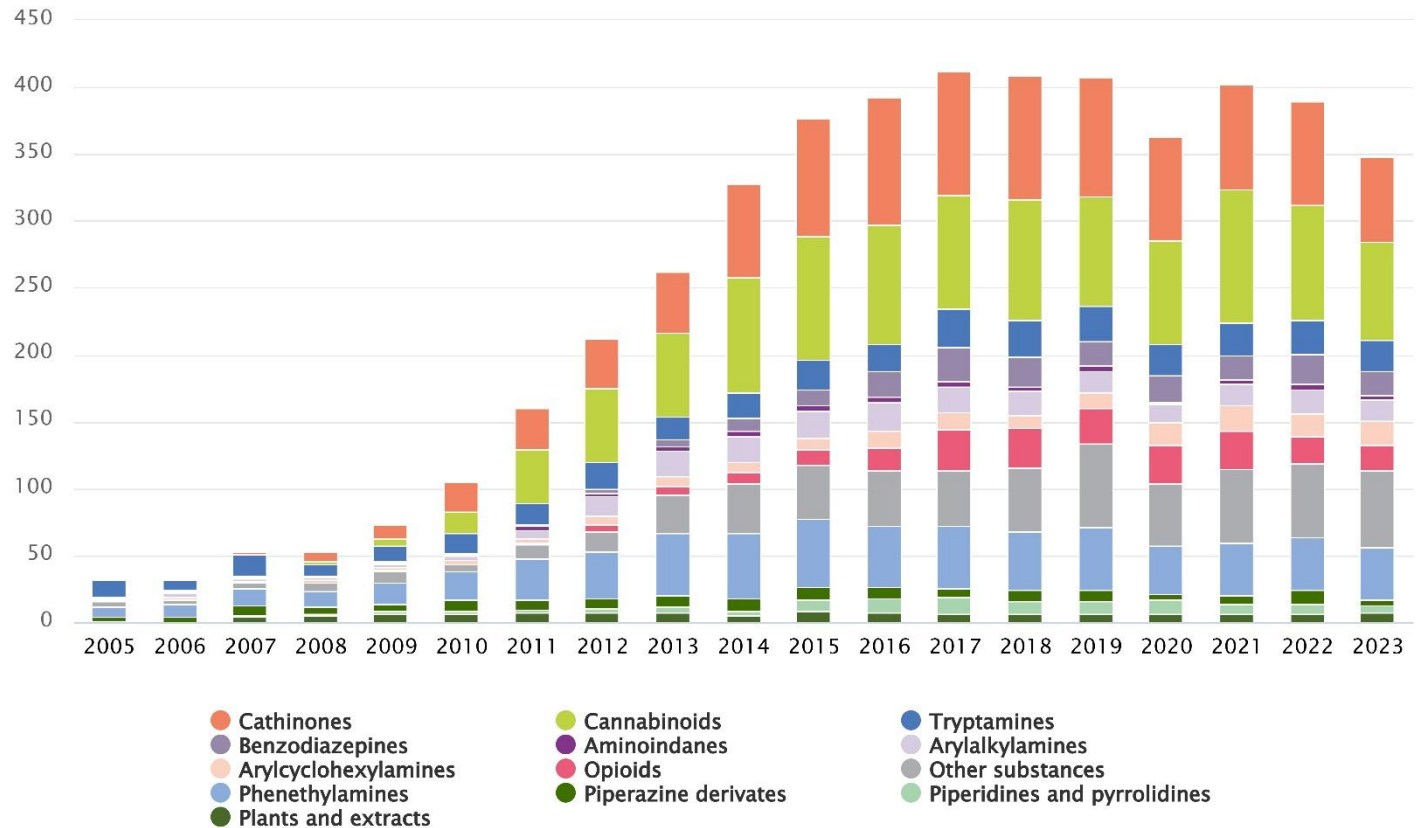
- Insgesamt **1000** NPS in EU 2024
- **47** erstmalig gemeldete Substanzen
- Und ca. **350** wiederkehrend



EUDA (data) | Highcharts (chart tool)

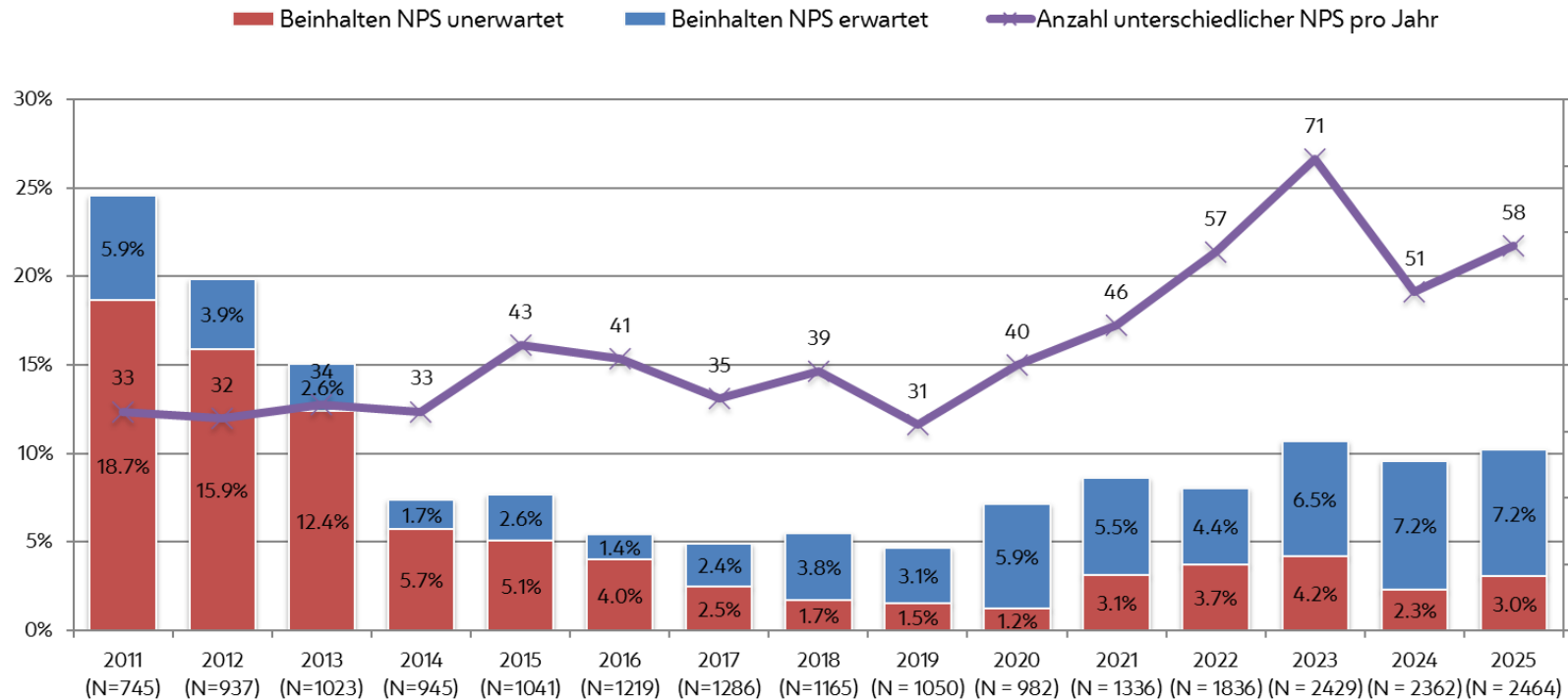
Neue Psychoaktive Substanzen – Aktuelle Situation

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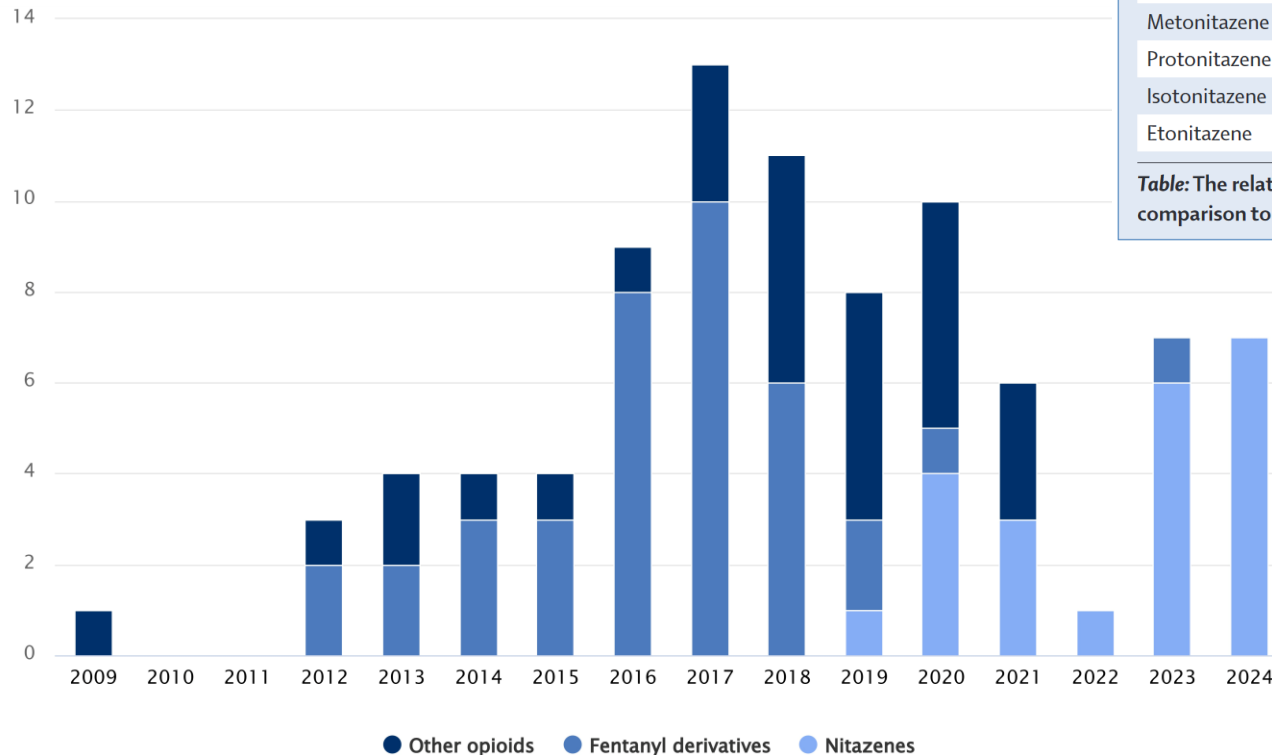
Neue Psychoaktive Substanzen – checkit! Wien



European Drug Report 2025, EUDA 2025

Neue Synthetische Opiode

Nitazene / Fentanyl



EUDA (data) | Highcharts (chart tool)

European Drug Report 2025, EUDA 2025

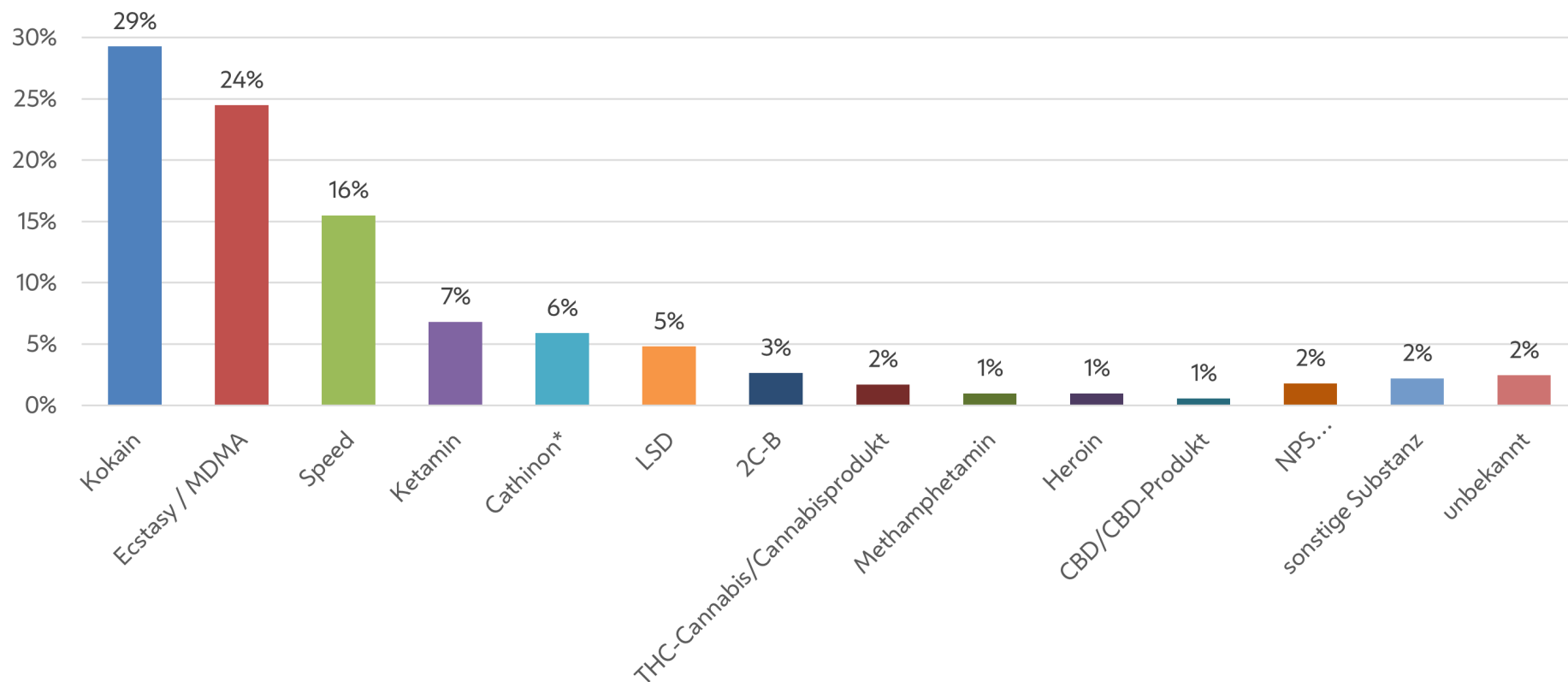
Relative potency to heroin	
Heroin	1
Fentanyl	50
Metonitazene	50
Protonitazene	100
Isotonitazene	250
Etonitazene	500

Table: The relative potency of fentanyl and selected nitazenes in comparison to heroin^{2,3}

Quelle: Holland et al. (2024)

Grund für Shift zu Nitazenen unklar. Generische Kontrollen von Fentanyl-Analoga in China (2019) & USA (2018) möglicherweise damit im Zusammenhang

Substanzen nach Abgabebezeichnung checkit! 2025



checkit!, Suchthilfe Wien gGmbH

Methoden zur Substanzanalyse (AKH Wien)

UHPLC-DAD



UHPLC-ITMS



MALDI-HRMS/MS



DSAP-ITMS



FTIR



Source: checkit! Suchthilfe Wien gmbH

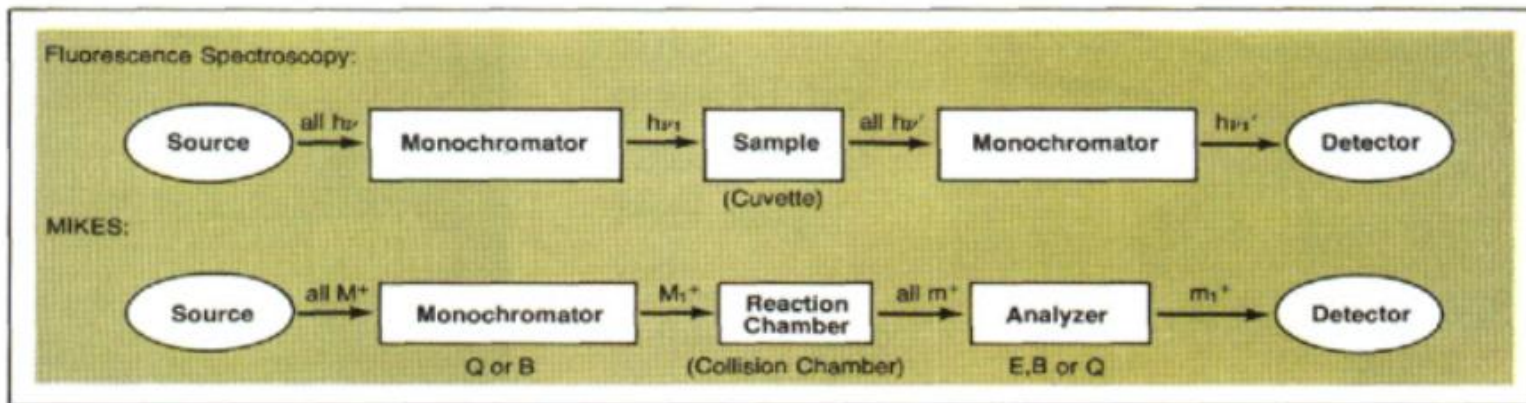
Direkte Massenspektrometrie

R. W. Kondrat and R. G. Cooks

Department of Chemistry
Purdue University
West Lafayette, Ind. 47907

Instrumentation

Direct Analysis of Mixtures by Mass Spectrometry



Scheme 1. Protocol for mixture analysis by MIKES as compared with similar steps involved in fluorescence spectroscopy

Direkte Massenspektrometrie

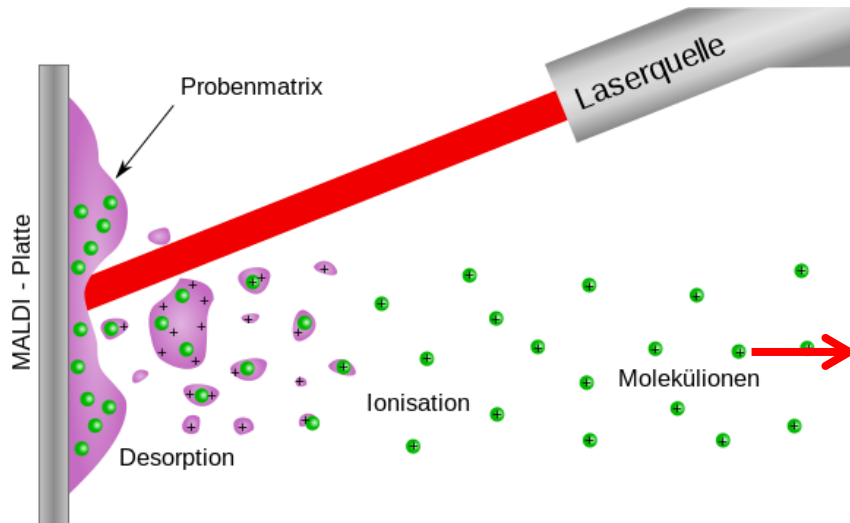
MALDI (Matrix Assisted Laser Desorption Ionization)



Foto: checkit! Suchthilfe Wien gGmbH

MALDI-MSⁿ – Prinzip

Ion Source:



Ion Trap MS:

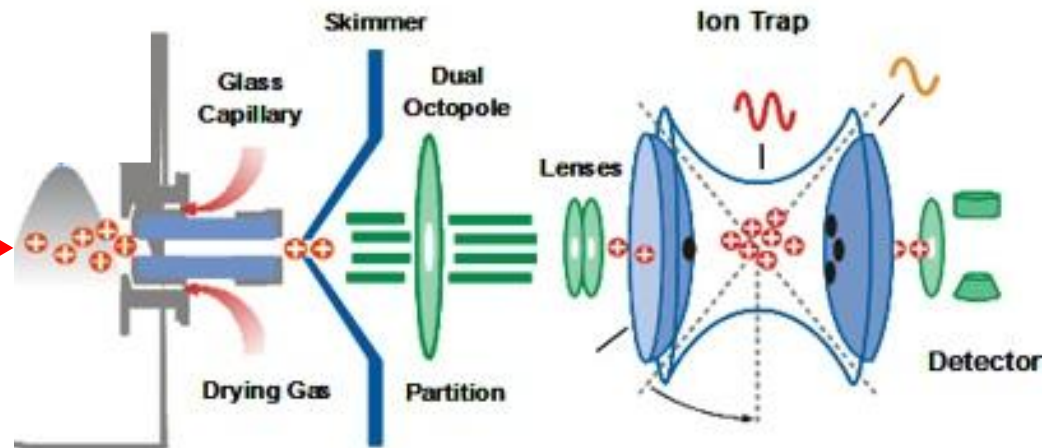
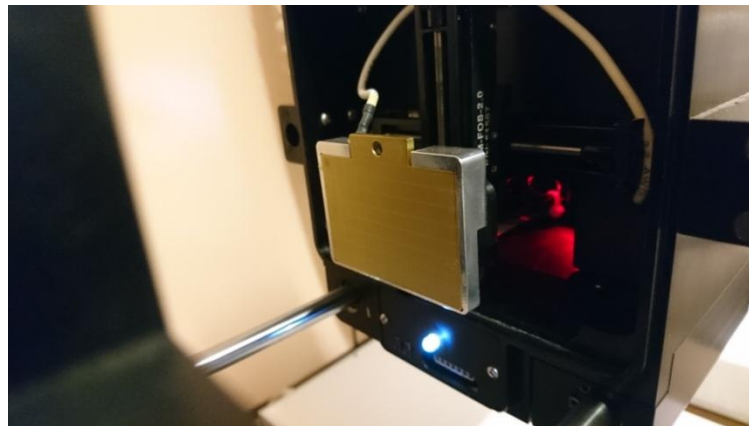
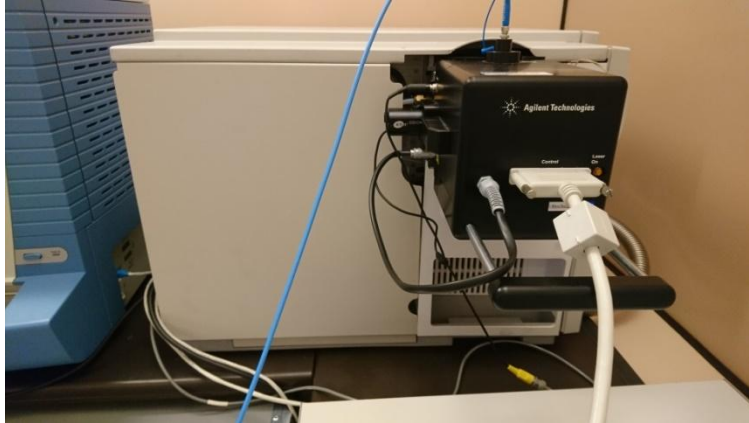


Bild Quelle: Mikayé - Eigenes Werk, CC BY-SA 3.0,
<https://commons.wikimedia.org/w/index.php?curid=25204006>

Direkte Massenspektrometrie

MALDI (Matrix Assisted Laser Desorption Ionization)

Direct MS: MALDI-IT-MSⁿ



Source: checkit! Suchthilfe Wien gGmbH

MALDI-Orbitrap - Probenvorbereitung

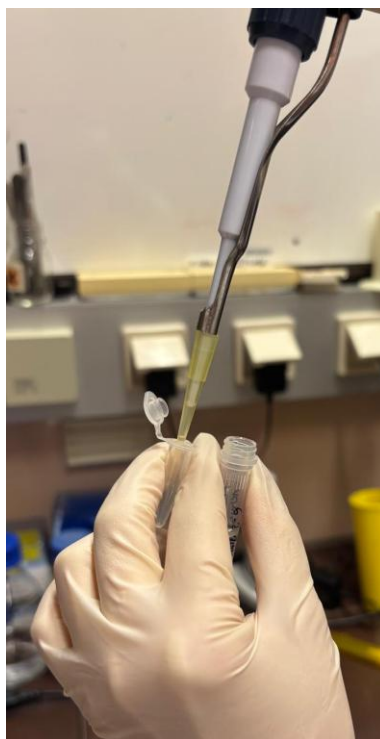
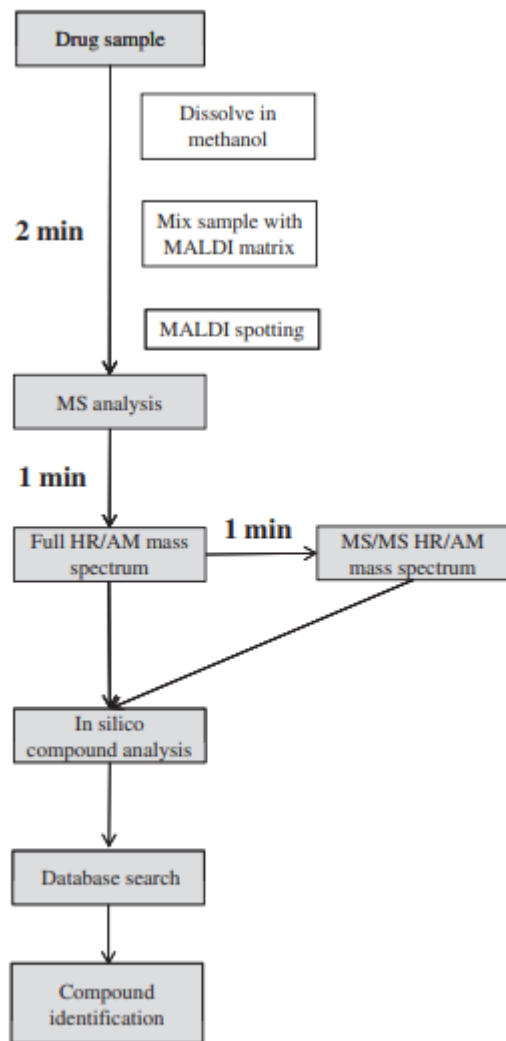
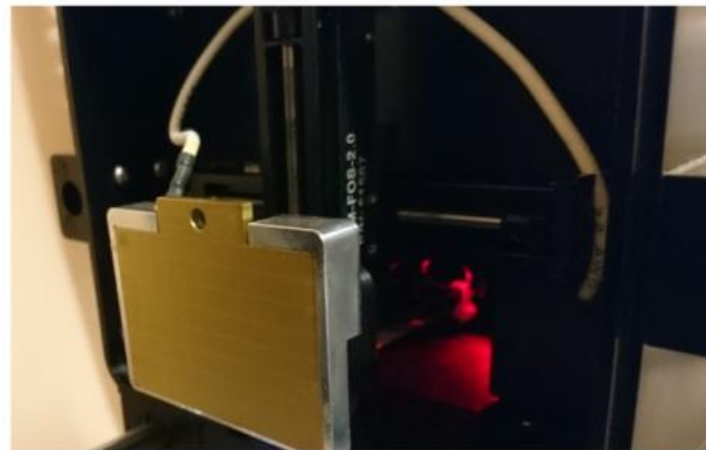
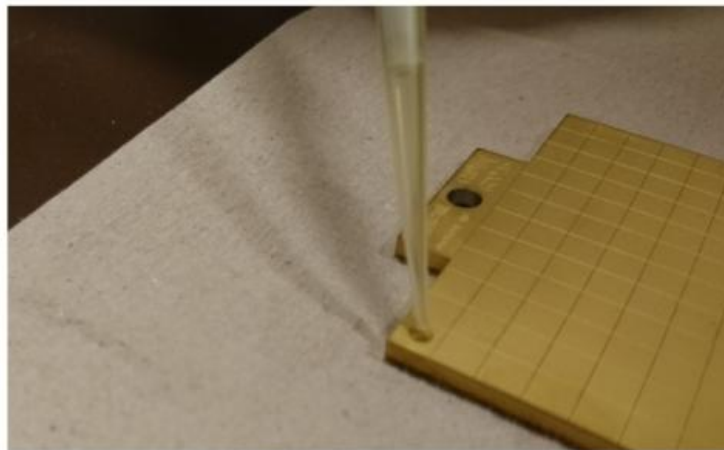


Fig. 1. Drug workup procedure and the following in silico compound analysis. MS, mass spectrometry; MALDI, matrix-assisted laser desorption/ionization; HR/AM, high resolution/accurate mass.

Source: Ostermann, Luf, Lutsch et. al, Clinica Chimica Acta, 2014

Direct MS: MALDI-IT-MSⁿ



Source: checkit! Suchthilfe Wien gGmbH

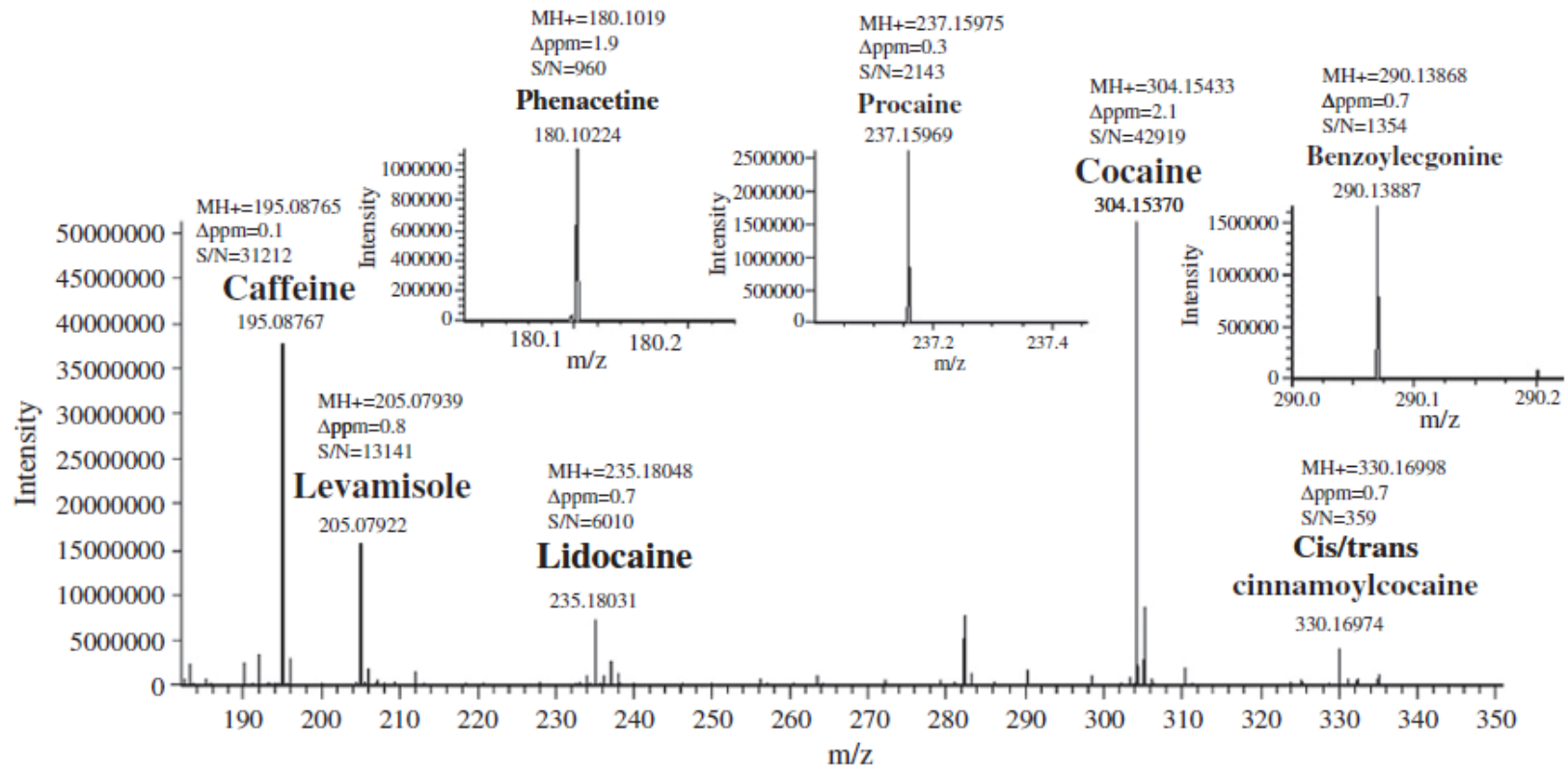


Source: checkit! Suchthilfe Wien gGmbH

UHPLC dilution & injection cycle with automated MALDI spotting

MALDI-Orbitrap – Beispielprobe

“Cocaine” sample



Source: Ostermann, Luf, Lutsch et. al, Clinica Chimica Acta, 2014

MALDI-Orbitrap 2025

Proof of Concept: Screening auf synthetische Opiode

Substanz	Parent Ion MALDI HRMS
Methoxyacetylfentanyl	353.1936
Para-chlorofentanyl	371.1585
Ocfentanyl	371.1822
Cyclopentylfentanyl	
Valeryl fentanyl	365.2291
Para-fluorobutyrylfentanyl	369.2034
Para-fluoro-methoxyacetylfentanyl	371.1829
Brorphine	400.1384
Butonitazene	425.2933
Etonitazepyne	395.2437
U-48800	343.1652
Fluonitazene	371.2216

- Data dependent Mass List Screening
- Tandem-MS (MS²)
- 311 Synthetische Opiode
- 12 Testsubstanzen in Mischung

MS2

CID

ITMS + p MALDI Full ms2 343.13@cid30.00 [65.00-355.00]

ITMS + p MALDI Full ms2 353.22@cid30.00 [70.00-365.00]

ITMS + p MALDI Full ms2 365.26@cid30.00 [70.00-380.00]

ITMS + p MALDI Full ms2 369.23@cid30.00 [75.00-380.00]

ITMS + p MALDI Full ms2 371.19@cid28.00 [75.00-385.00]

ITMS + p MALDI Full ms2 371.21@cid30.00 [75.00-385.00]

ITMS + p MALDI Full ms2 377.26@cid30.00 [75.00-390.00]

ITMS + p MALDI Full ms2 395.21@cid26.00 [80.00-410.00]

ITMS + p MALDI Full ms2 400.00@cid28.00 [80.00-410.00]

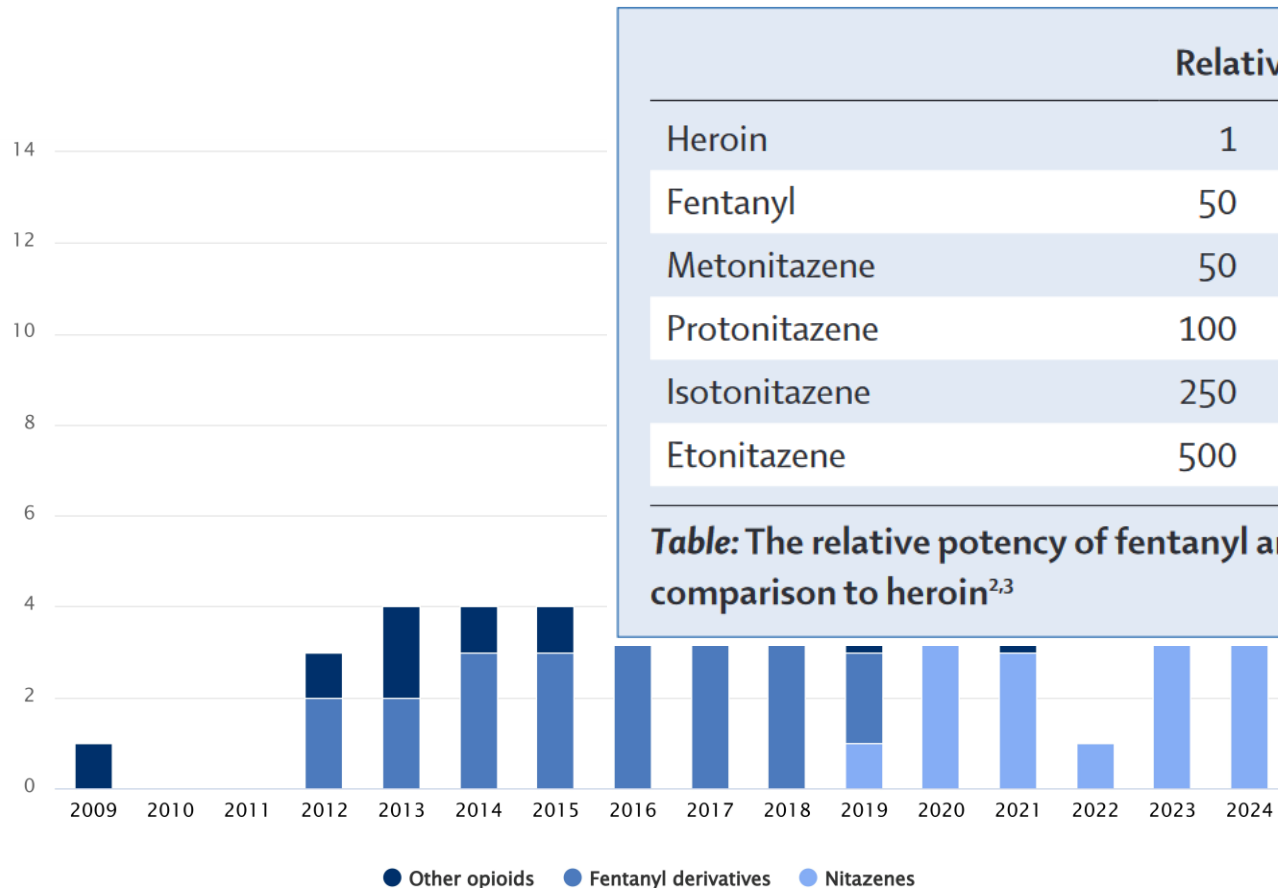
ITMS + p MALDI Full ms2 425.25@cid26.00 [85.00-440.00]

Figure 20: MS² profiling of novel synthetic opioids on the MALDI-Orbitrap XL.
Ion-Trap CID parameters and precursor mass selection for reliable fragmentation

Source: Masterarbeit, Simona Aigner, 2025 (modifiziert)

Neue Synthetische Opiode

Nitazene / Fentanyle



Relative potency to heroin

Heroin	1
Fentanyl	50
Metonitazene	50
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Etonitazene	500

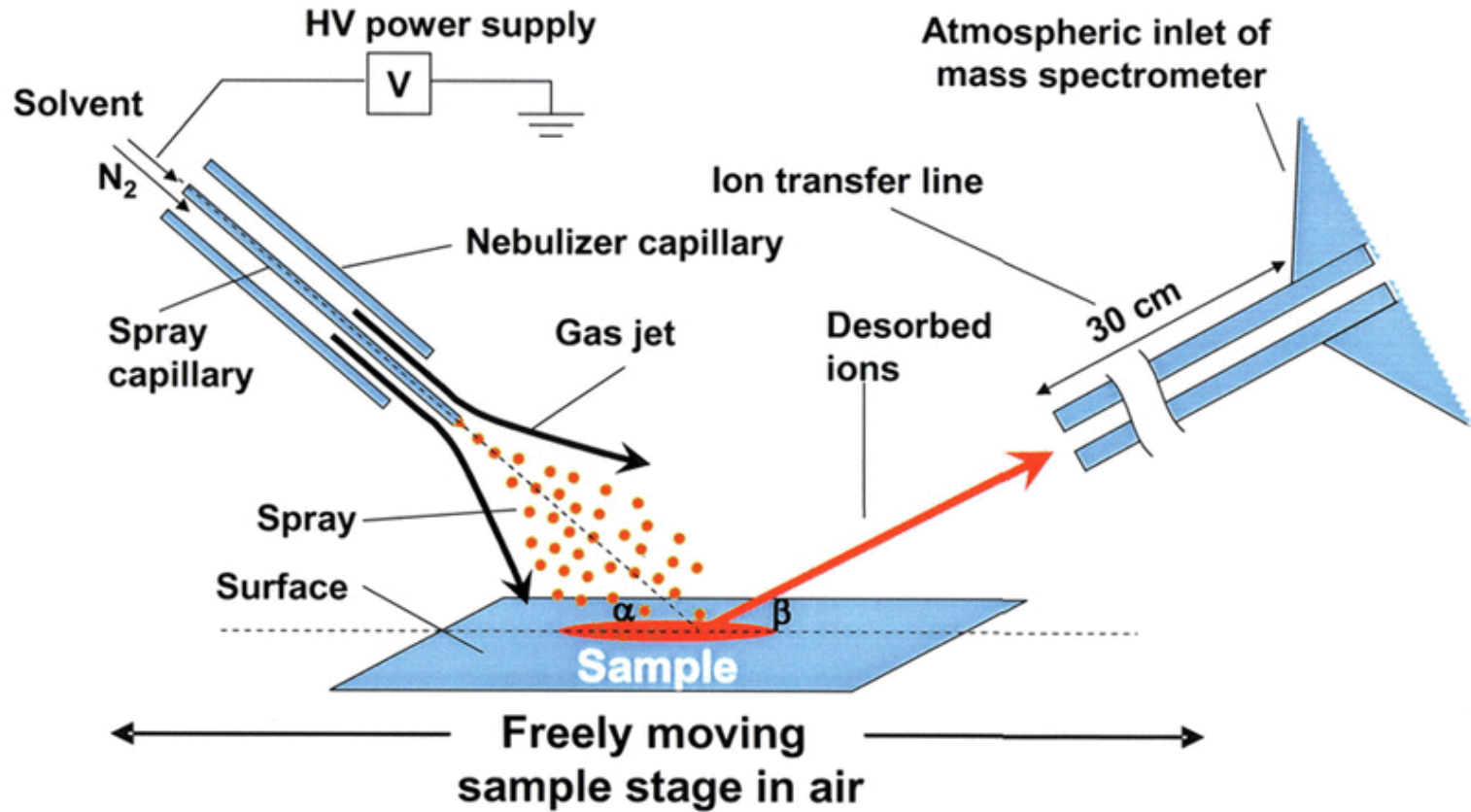
Table: The relative potency of fentanyl and selected nitazenes in comparison to heroin^{2,3}

von Fentanyl-Analoga in China (2019) & USA (2018) möglicherweise damit im Zusammenhang

EUDA (data) | Highcharts (chart tool)

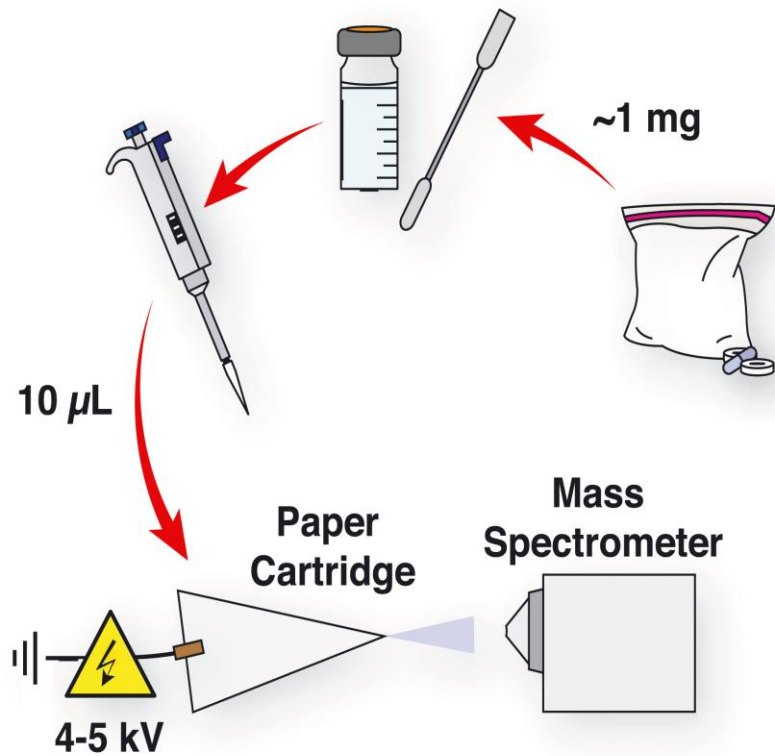
European Drug Report 2025, EUDA 2025

DESI (Desorption Electrospray Ionisation)



Takats et al. 2004, Science, Mass Spectrometry Sampling Under Ambient Conditions with Desorption Electrospray Ionization

Paper Spray Ionisation

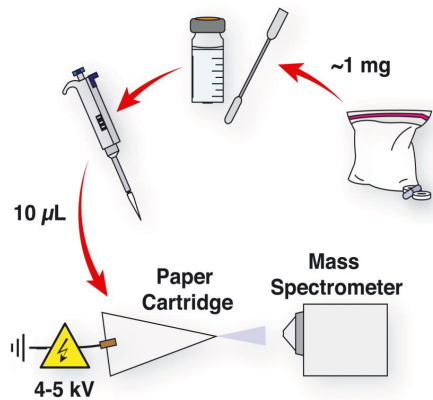


**Journal of Mass Spectrometry, Volume: 54, Issue: 9,
Pages: 729-737, First published: 20 August 2019, DOI:
(10.1002/jms.4431)**

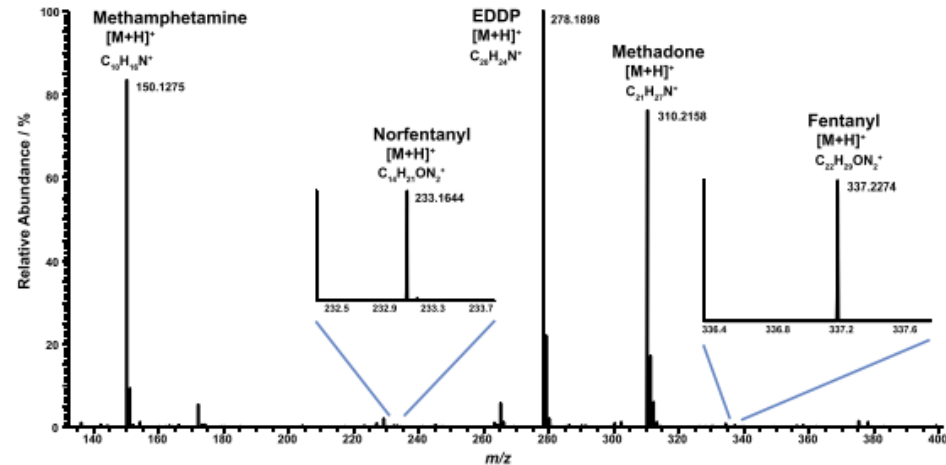


J. Braz. Chem. Soc. 32 (2) • Feb 2021
<https://doi.org/10.21577/0103-5053.20200177>

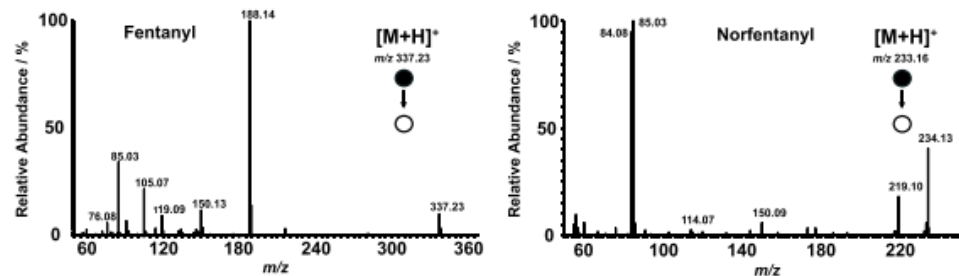
Paper Spray Ionisation



High-Resolution Mass Spectrometry (Sample Characterization)

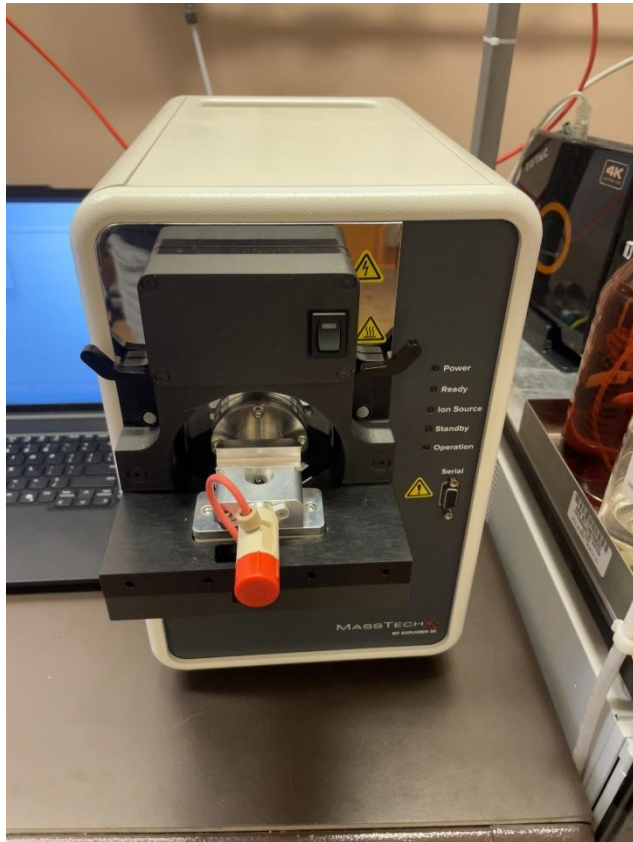


Tandem Mass Spectrometry (Identity Confirmation)



Journal of Mass Spectrometry, Volume: 54, Issue: 9, Pages: 729-737, First published: 20 August 2019, DOI: (10.1002/jms.4431)

MTE-30 – Miniatur-Ionenfalle



- 3-D-Ionenfalle
- Gewicht: 17 Kg
- Collision gas: Wasserstoff
- Batteriebetrieben (optional)
- Fragmentierung bis MS^3



DSAP-Quelle

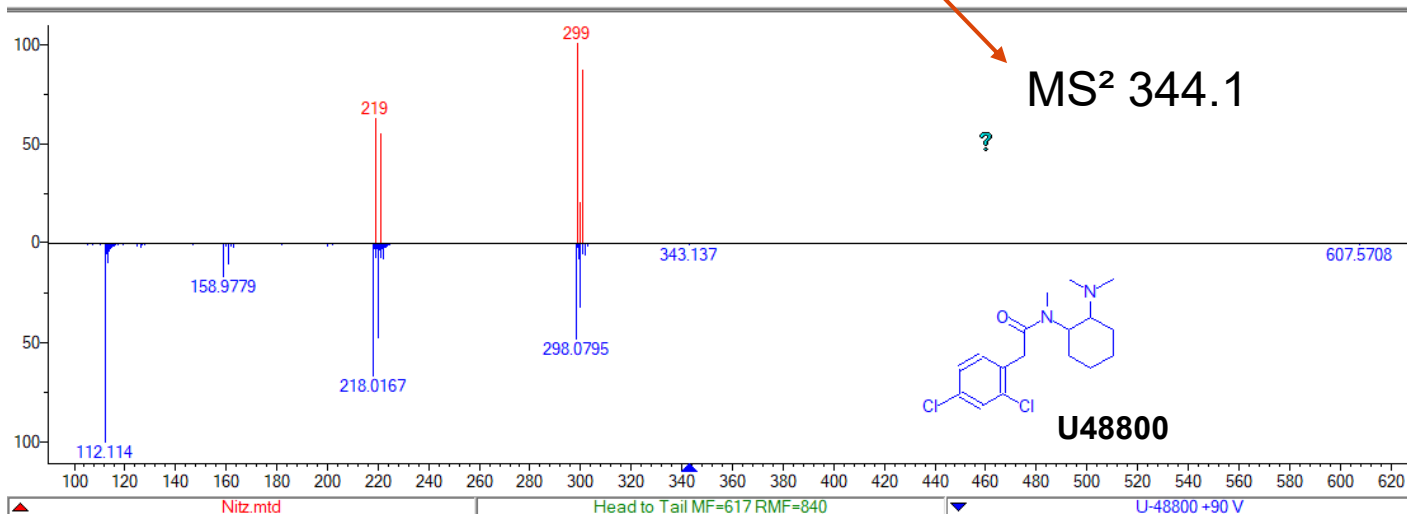
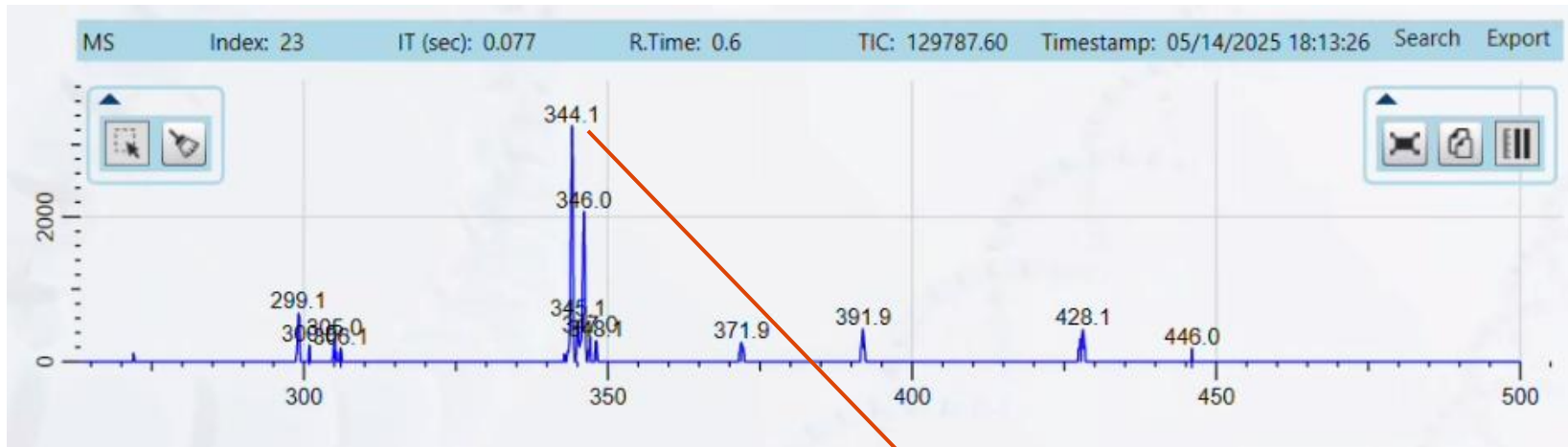


LSADP-Quelle

Source: checkit! Suchthilfe Wien gGmbH

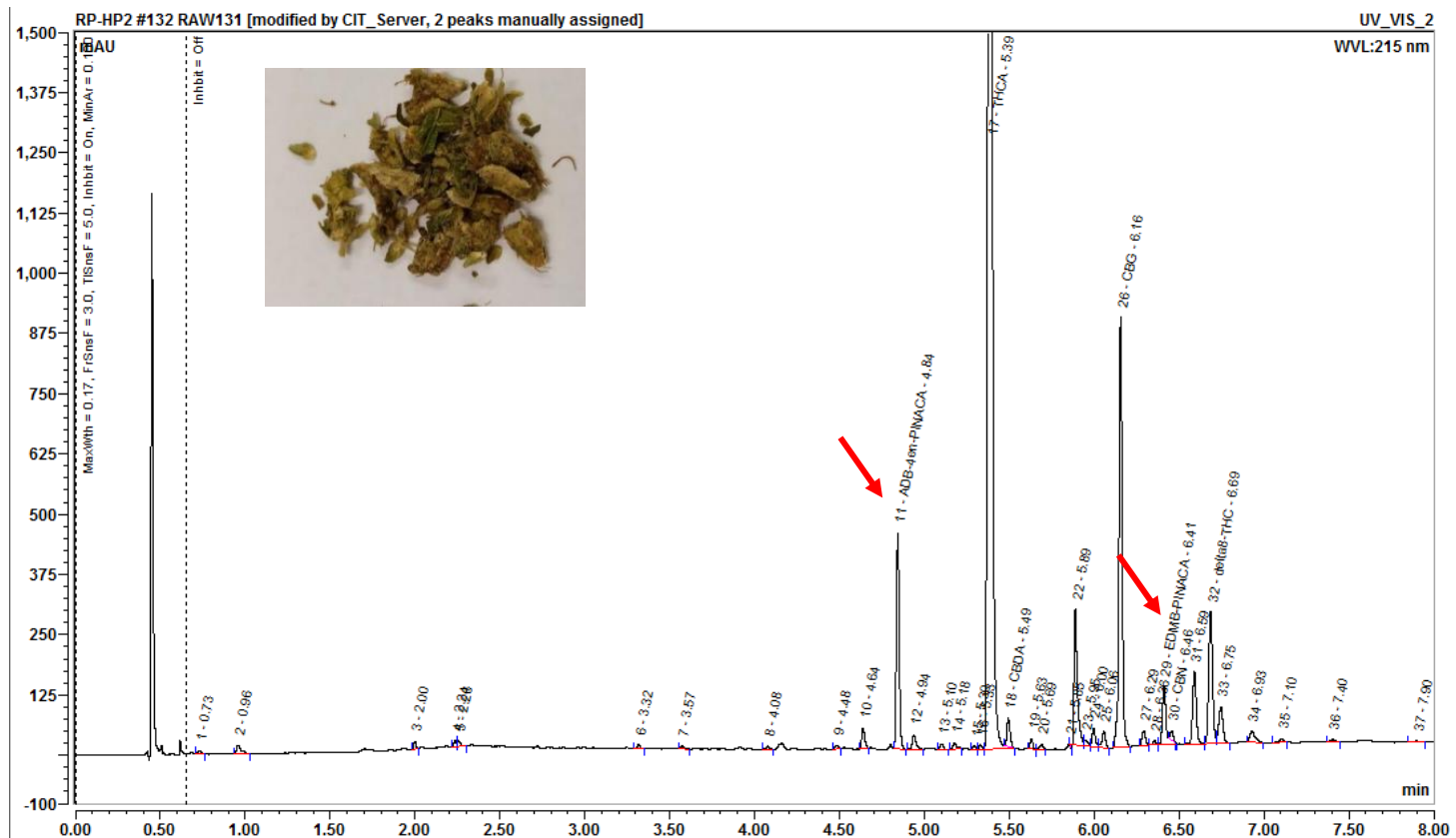
MTE-30 – Miniatur-Ionenfalle

Synthetische Opioide: Testmischung



Source: checkit! Suchthilfe Wien
gGmbHc

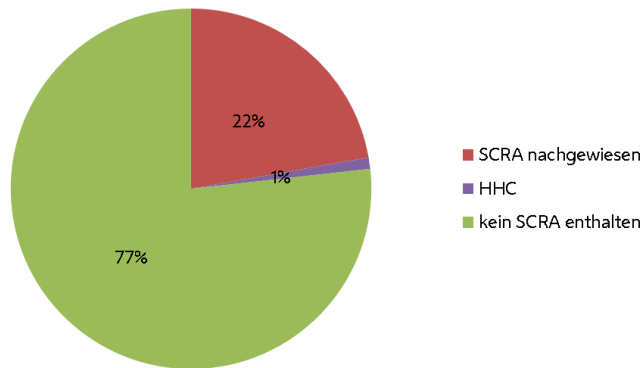
Challenges – High number of SCRA



Source: checkit! Suchthilfe Wien gGmbH

checkit! – Analyseergebnisse von Verdachtsproben

Ergebnisse der Analyse von Proben mit Verdacht auf
synthetische Cannabinoide
Januar 2022 - Ende Dezember 2022
n = 99

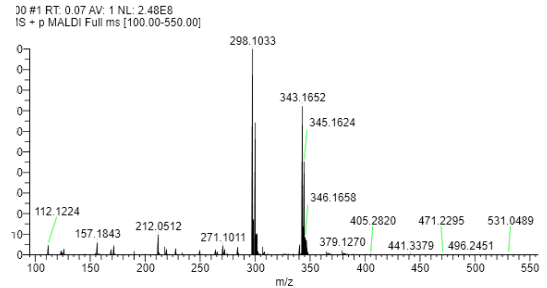
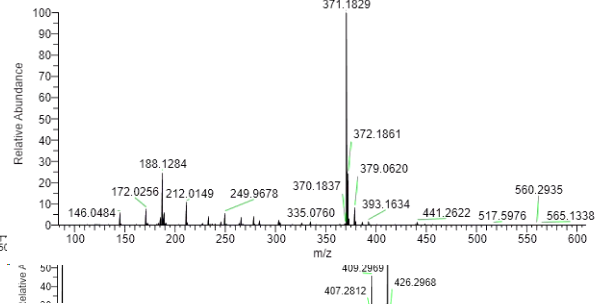
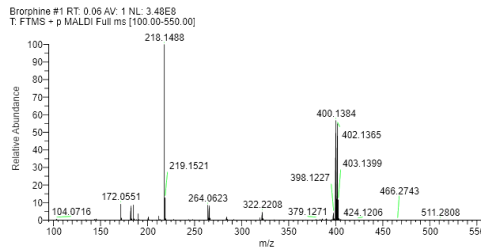


Quelle: checkit!, Suchthilfe Wien gGmbH

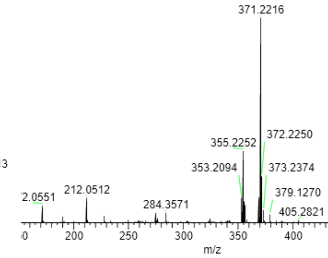
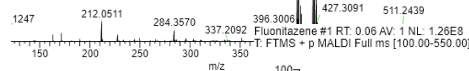
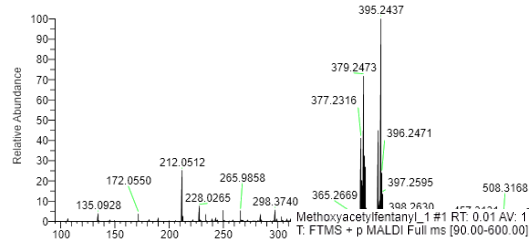
abgegeben als	Anzahl	davon mit SCRA/HHC
Damiana	1	1
Cannabis	86	20
Haschisch	4	1
THC-Extrakt	2	0
THC-Edible	1	0
THC-Liquid	2	0
CBD	2	0
HHC	1	1
Ergebnis	99	23

Datenauswertung??

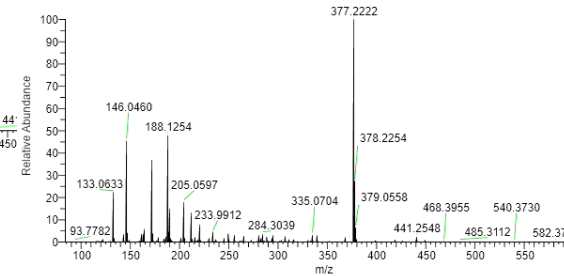
para-fluoro-Methoxyacetylfentanyl_1 #1 RT: 0.06 AV: 1 NL: 4.74E7
T: FTMS + p MALDI Full ms [100.00-550.00]



Etionitazepine #1 RT: 0.06 AV: 1 NL: 1.95E8
T: FTMS + p MALDI Full ms [100.00-550.00]



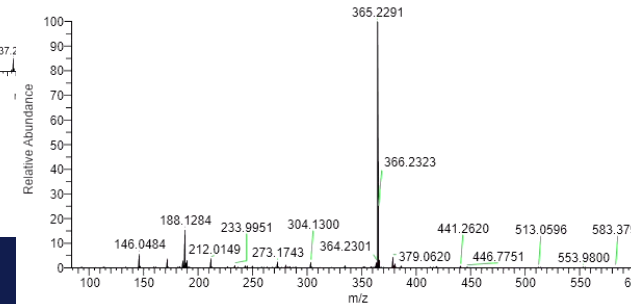
Cyclopentylfentanyl #23 RT: 1.57 AV: 1 NL: 1.36E7
T: FTMS + p MALDI Full ms [90.00-600.00]



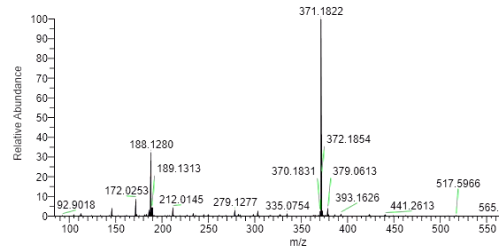
para-Chlorofentanyl_1 #1 RT: 0.01 AV: 1 NL: 4.56E7
T: FTMS + p MALDI Full ms [90.00-600.00]



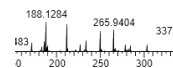
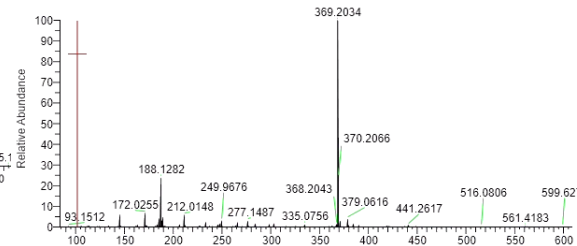
Valeryl-fentanyl_1 #1 RT: 0.01 AV: 1 NL: 4.90E7
T: FTMS + p MALDI Full ms [90.00-600.00]



Ocfentanil_1 #1 RT: 0.01 AV: 1 NL: 8.20E7
T: FTMS + p MALDI Full ms [90.00-600.00]

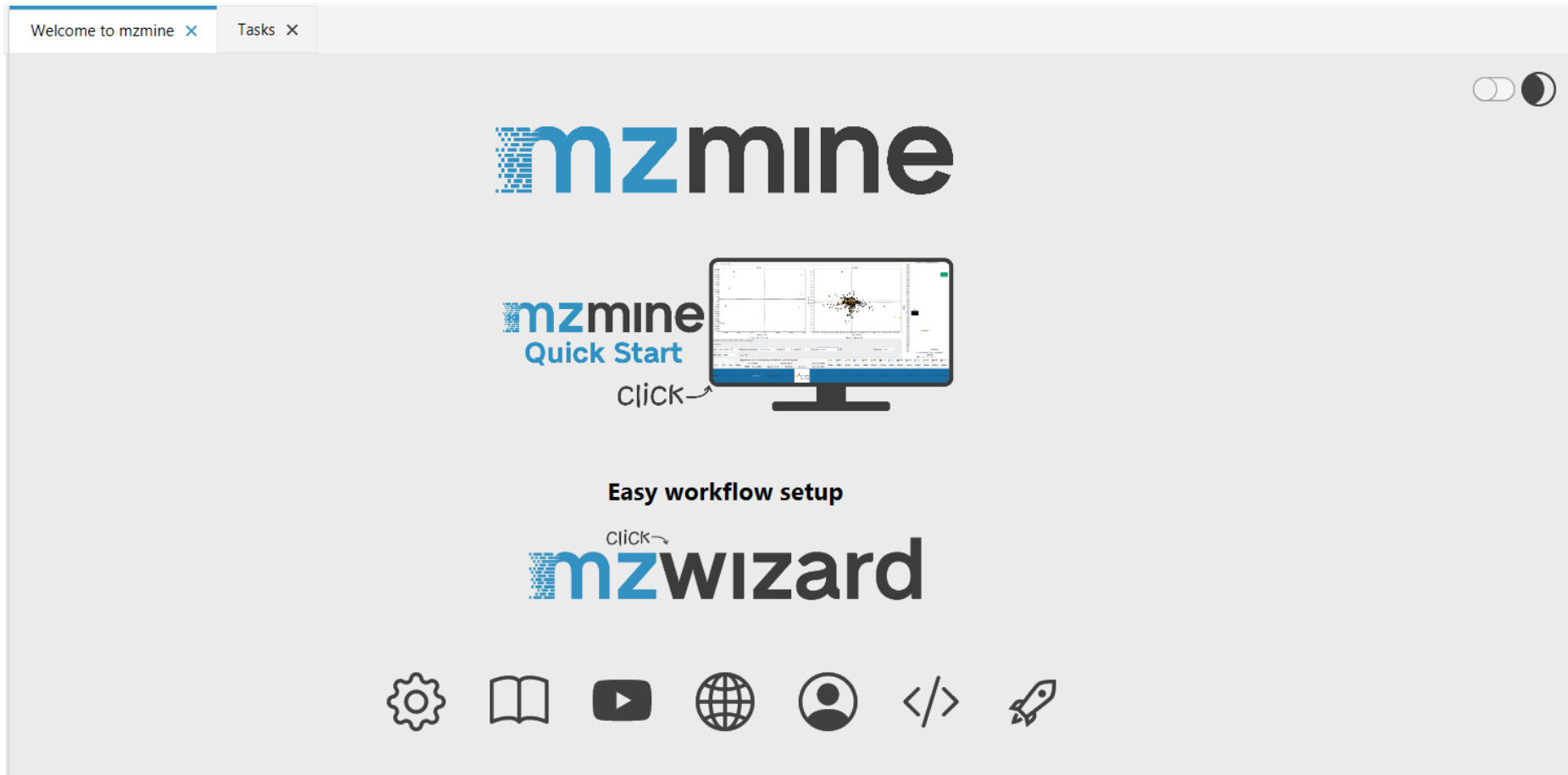


para-Fluorobutylfentanyl_1 #1 RT: 0.07 AV: 1 NL: 5.15E7
T: FTMS + p MALDI Full ms [90.00-600.00]



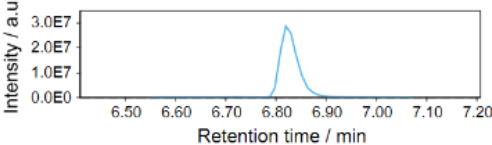
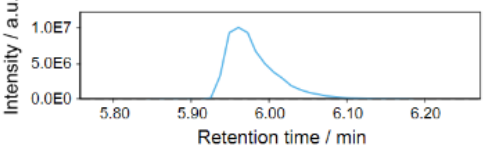
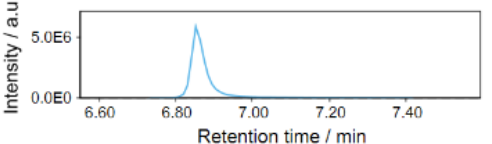
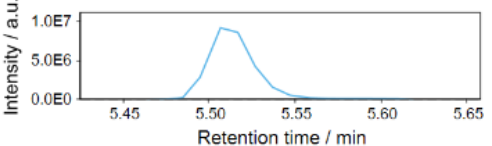
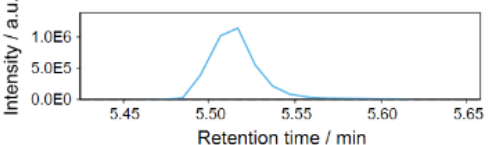
Source: checkit! Suchthilfe Wien gGmbHc

Datenauswertung - Automatisierung



Schmid, R., Heuckeroth, S., Korf, A. *et al.* Integrative analysis of multimodal mass spectrometry data in MZmine 3. *Nat Biotechnol* **41**, 447–449 (2023). <https://doi.org/10.1038/s41587-023-01690-2>

Datenauswertung - Automatisierung

					A12_2			
m/z	RT	Area	Height	Comment	Shapes	Preferred Annotat		
						Preferred Annotation ▼	AQS	Formula
315.2801	6.82	1.4E6	2.9E7			CBD (0.855)		C21H30O2
359.2512	5.96	6.7E5	1.0E7			.beta.'-Hydroxythiofentanyl +60 V (0.732)		C20H26N2O2S
329.2447	6.85	3.1E5	6.0E6			1^''6a(10a)-Tetrahydrocannabiol +60 V (0.712)		C21H30O2
341.2618	5.51	3.0E5	9.3E6			para-Fluorocetyl fentanyl +30 V (0.686)		C21H25FN2O
359.2436	5.52	3.9E4	1.2E6			Cannabidiolic Acid Methyl Ester +60 V (0.660)		C23H32O4

Methodenentwicklung und aktuelle Spektrendatenbanken notwendig

Source: checkit! Suchhilfe Wien gGmbHc

Direkte Massenspektrometrie - Fazit

Direkte Massenspektrometrische Methoden (DESI, MALDI, DART, PSI etc.)

Potentiale:

- Einfache Anwendung
- Hoher Probendurchsatz
- Eignung für schnelle Screeningverfahren (MRM/SRM Methoden)
- Minimale Probenvorbereitung
- “Sanfte Ionisation”
- Hohe Sensitivität

Limitierungen:

- Keine chromatographische Trennung (Vielstoffgemische)
- Selektivität: Positionsisomere, Isobare etc. oft nicht differenzierbar
- Matrixeffekte und ion-suppression
- Quantifizierung störanfällig
- Hoher technischer Aufwand

→ Kombination komplementärer Analyseverfahren notwendig!

Danke!



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alexander.lantzberg@meduniwien.ac.at