# Expanding Analytical Frontiers: Showcasing the Portability and Versatility of Miniature Ion Trap Mass Spectrometry

Presented by Caleigh O'Connor

*With special thanks to Vladimir Doroshenko, Nivedita Bhattacharya, Venkat Panchagnula, Enrico Davoli, Nitin Karalkar, and Victor Laiko*

# Portability

# Diverse Ion Source Options


Mini HPLC

*Axcend Focus LC*



Nano-ESI

*ThermoFisher*



ESI

*MassTech*



APCI

*MassTech*



SICRIT

*Plasmion*

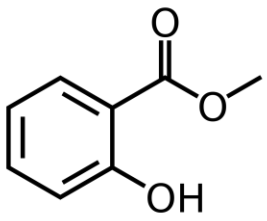


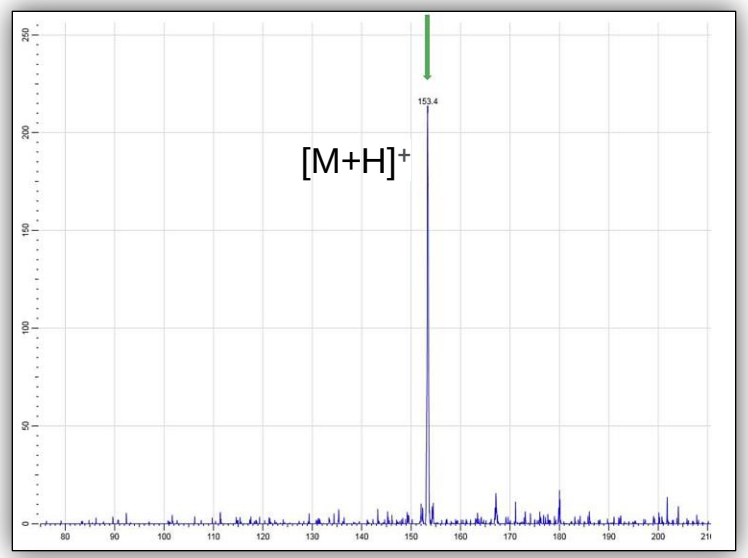
LDSAP

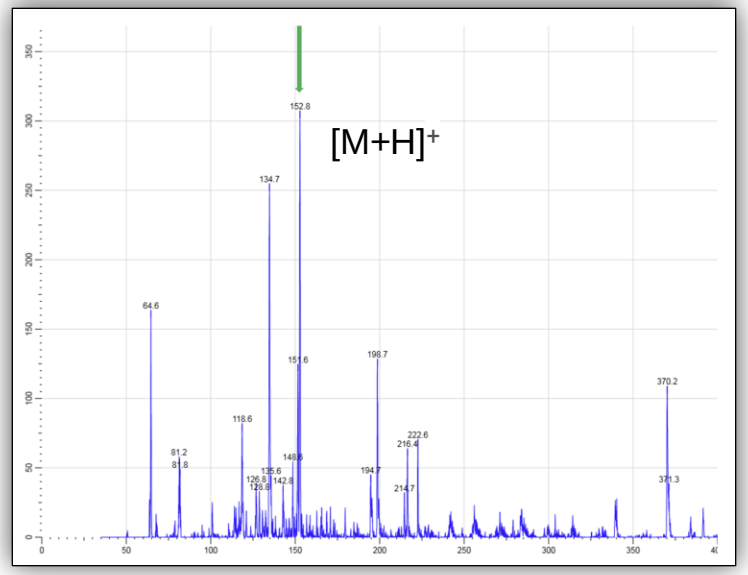
*MassTech*

# Forensics: Hazardous Substances

Methyl Salicylate

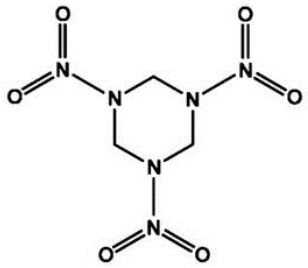


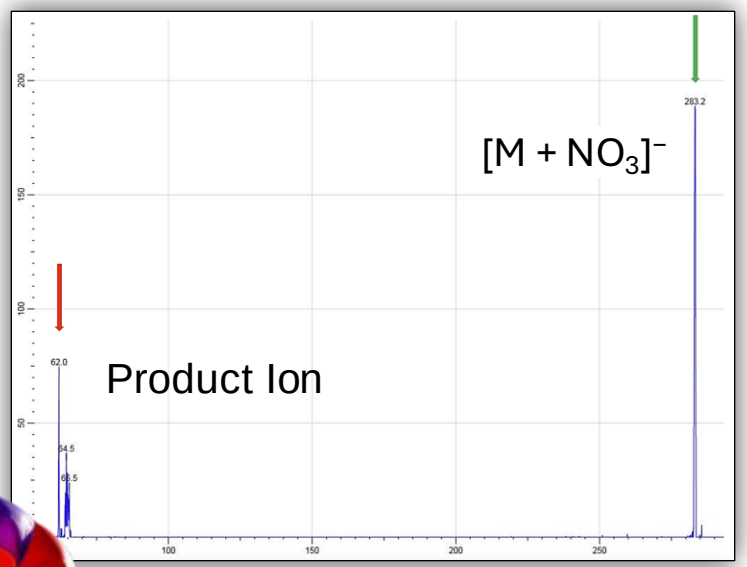



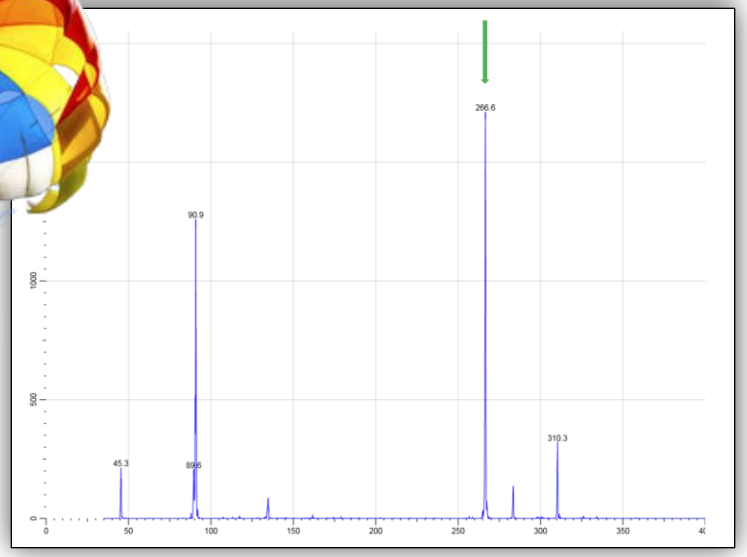




*Top: SICRIT® GC/SME-MS of 500 pg methyl salicylate, a CWA simulant.*
*Bottom: APCI-MS of 2 ng methyl salicylate*

RDX



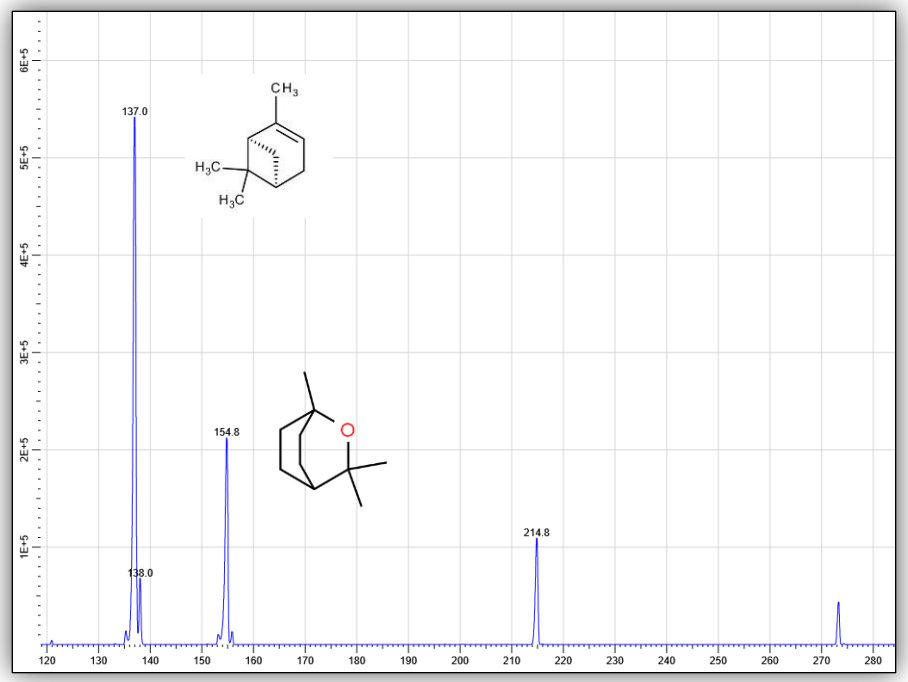




*Top: SICRIT® GC/SME-MS of 2 ng sample of RDX explosive*
*Bottom: APCI-MS of 2 ng RDX (negative ion mode)*

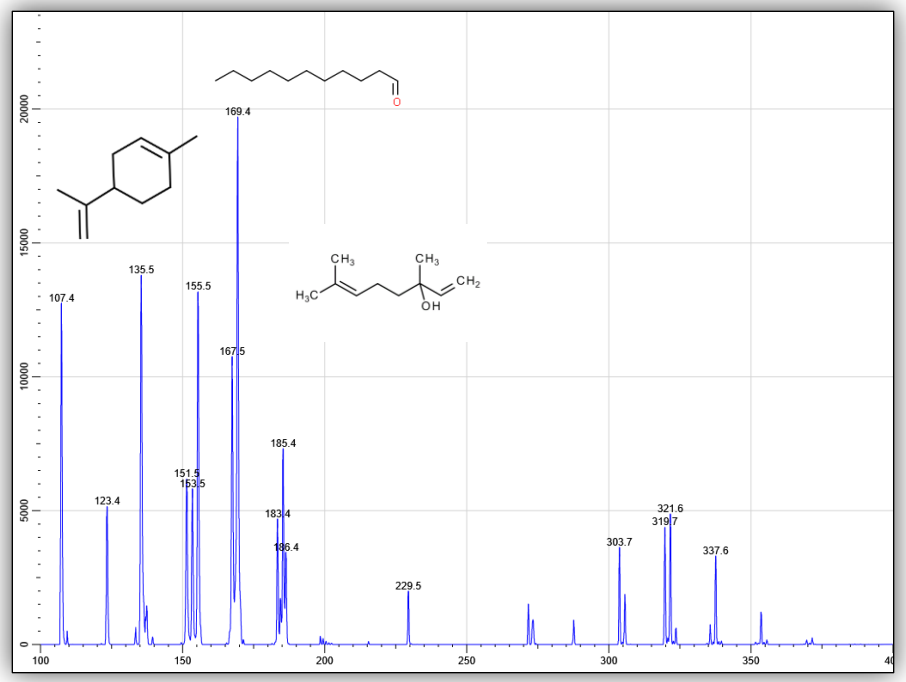
# Ambient Conditions Monitoring


## Eucalyptus Essential Oil




*"APCI"-MS of Eucalyptus essential oil in methanol on a swab in proximity to the needle. Molecule assignments are proposed.*

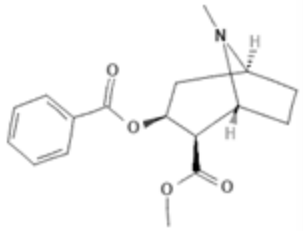
## Sweet Orange Essential Oil

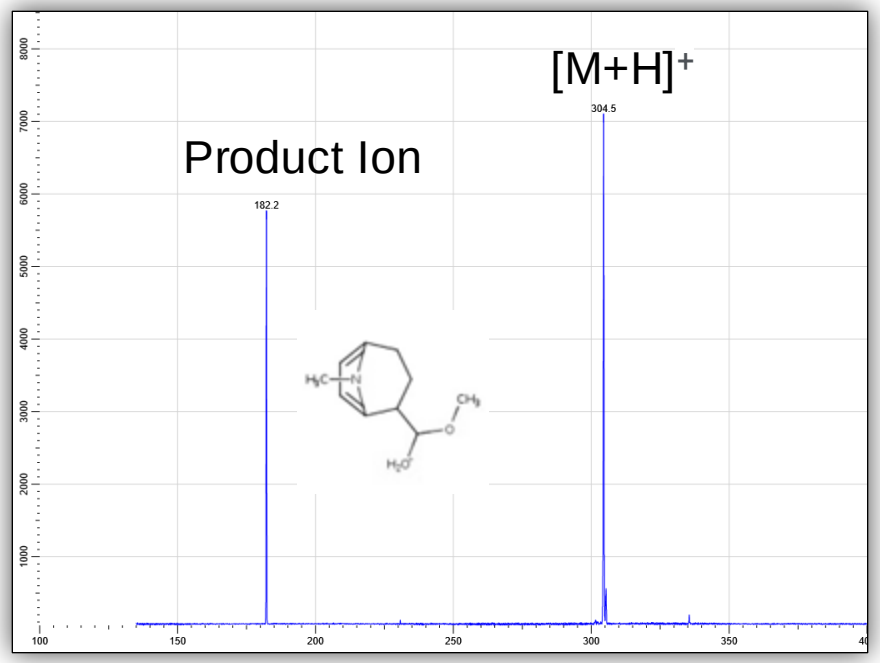



*"APCI"-MS of Sweet orange essential oil in methanol on a swab in proximity to the needle. Molecule assignments are proposed.*

# Forensics: Drugs of Abuse

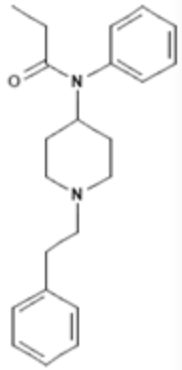
## Cocaine

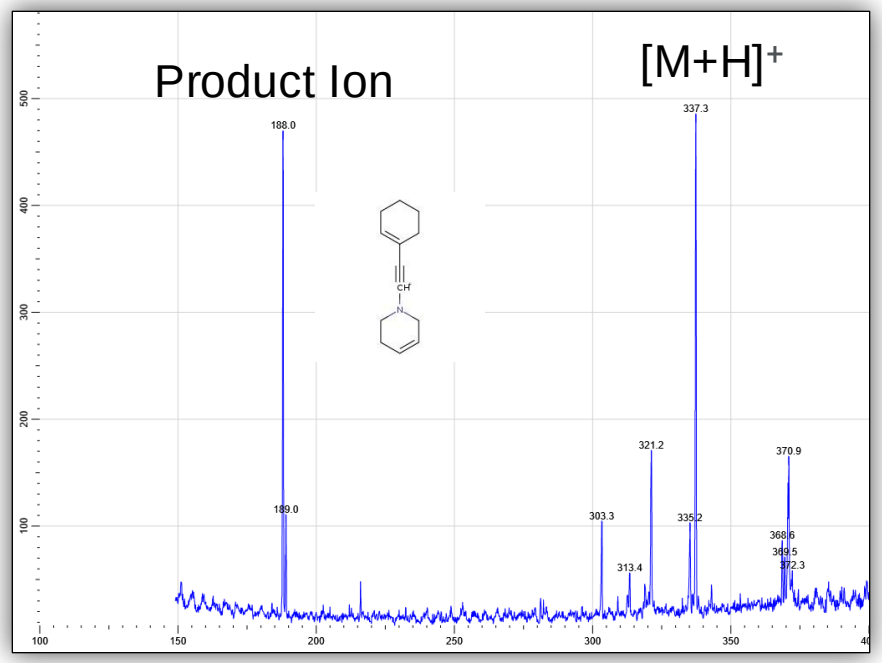





*ESI-MS/MS of 100ng/mL cocaine in synthetic urine after BioSPME treatment. Parent ion (304 m/z) and major fragment (182 m/z) shown. Fragment structure proposed by CFM-ID*

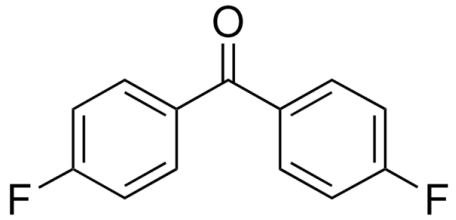
## Fentanyl



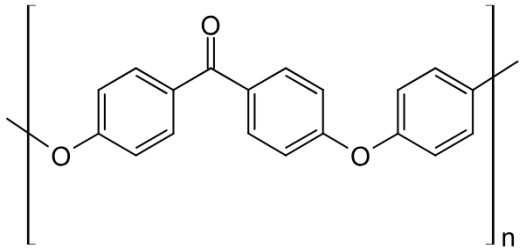


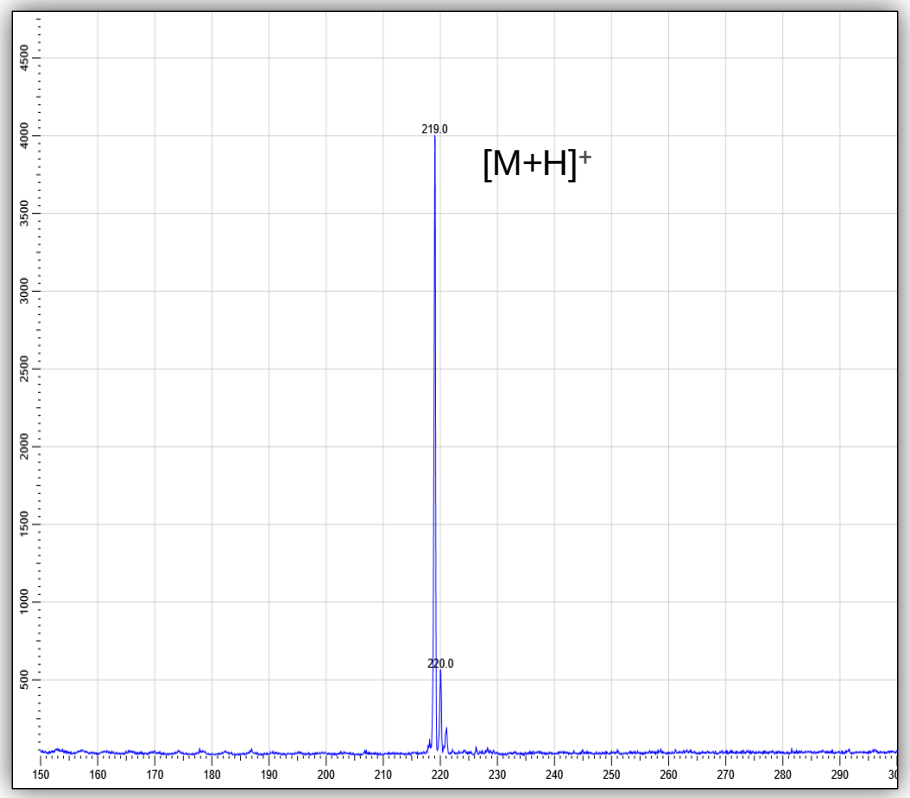

*ESI-MS/MS of 10ppb of fentanyl. Parent ion 337 m/z, major fragment 188 m/z. Fragment structure proposed by CFM-ID*

# Materials Manufacturing Monitoring

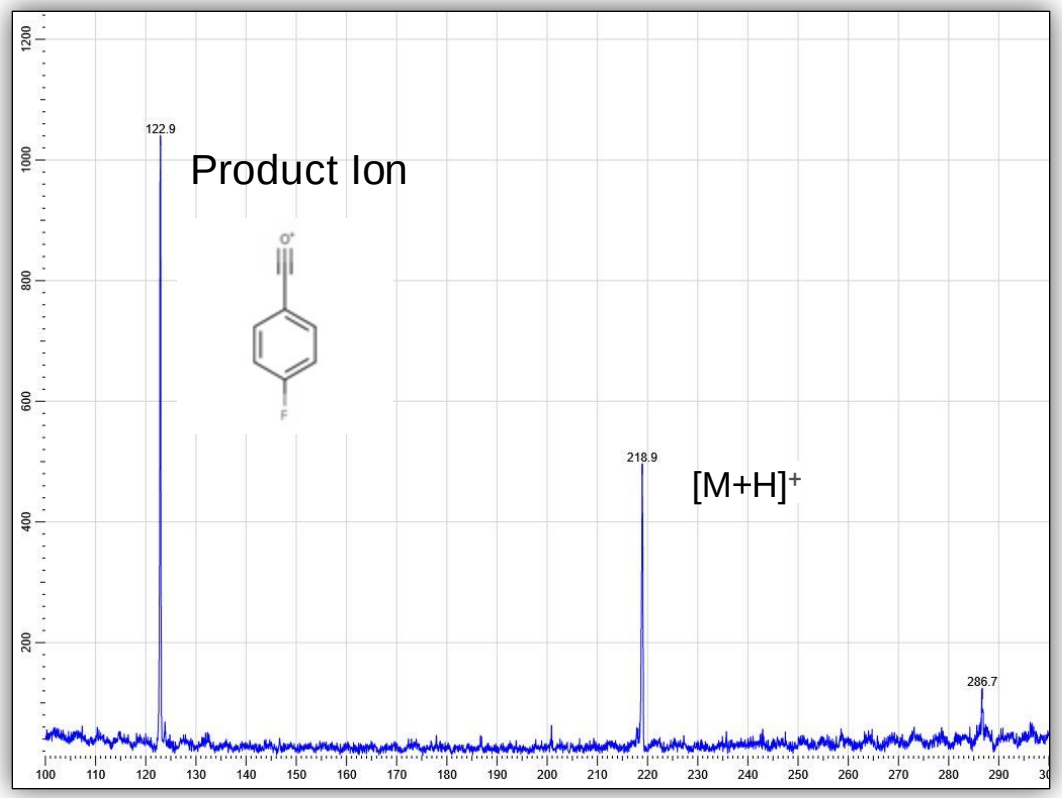



4,4’-Difluorobenzophenone (PEEK precursor)



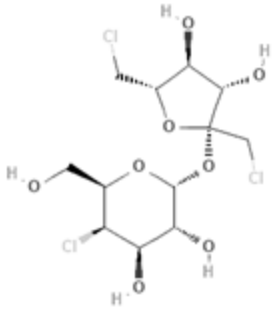

*ESI-MS/MS isolation of 100 µg/mL 4,4'-Difluorobenzophenone—a PEEK precursor*

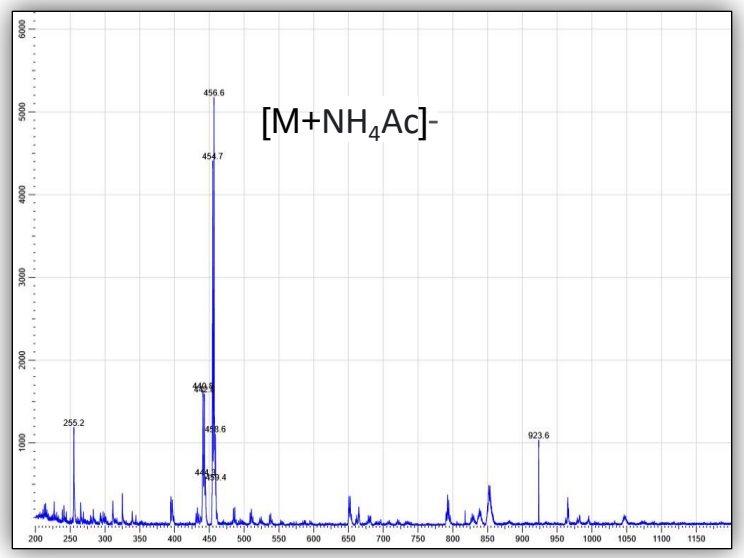



*ESI-MS/MS fragmentation of 100 µg/mL 4,4'-Difluorobenzophenone. Parent ion 218 m/z, major fragment 122 m/z (structure is proposed by CFM-ID)*

# Small Molecules and Pharma

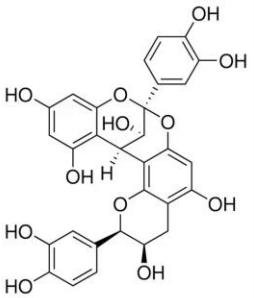
## Sucralose

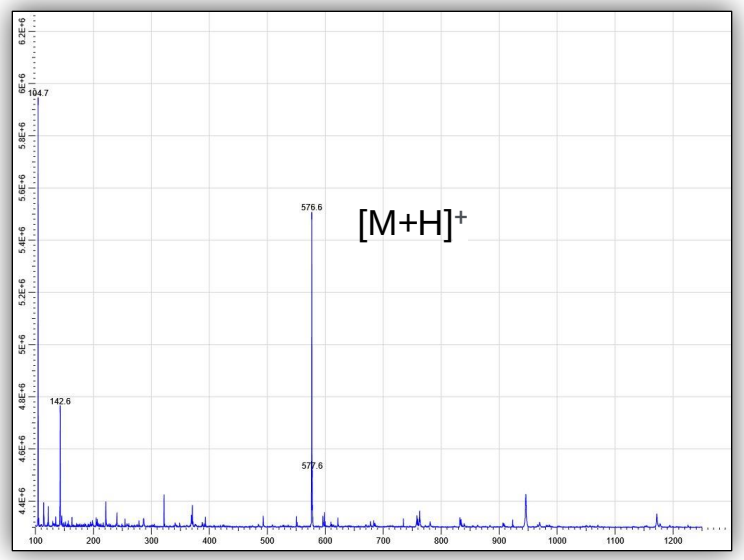





*ESI-MS of µg/mL sucralose sample—peak may represent the ammonium acetate adduct obtained in negative ion mode*

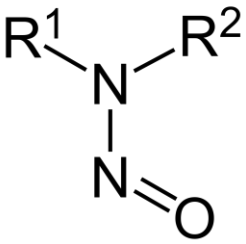
## Procyanidin A2

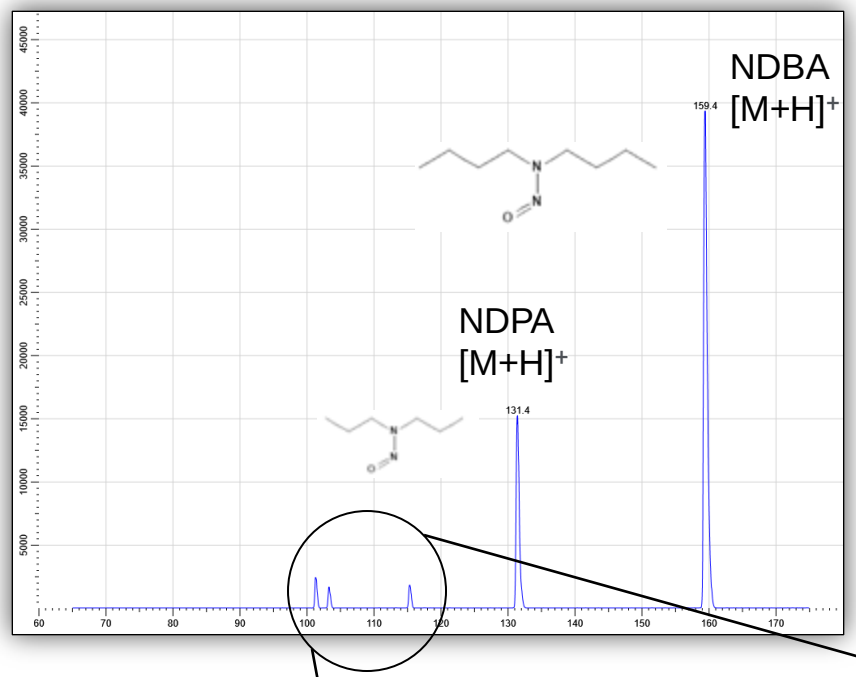


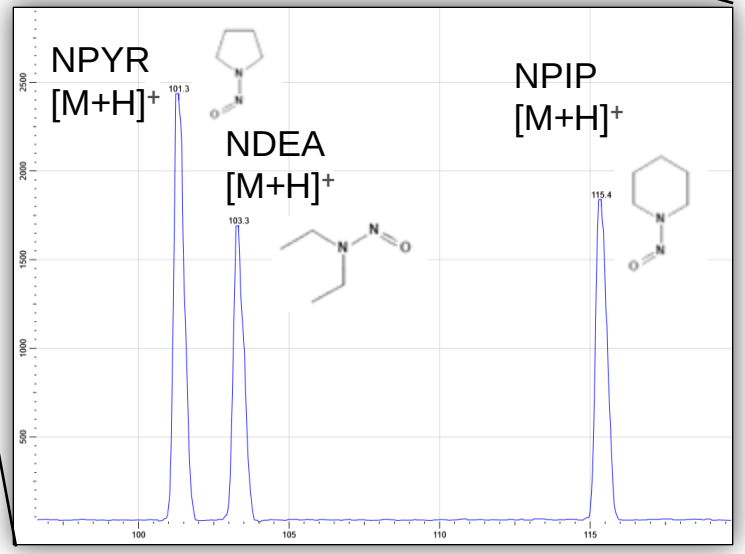



*ESI-MS of 100 µg/mL Procyanidin A2 (flavonoid in grape, avocado, cranberry juice, etc)*

## 7-Nitrosamine Mix

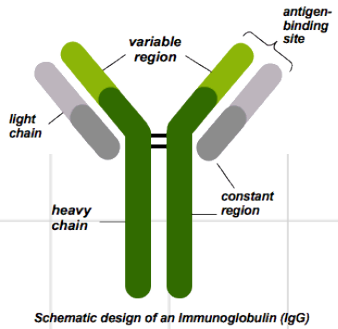



*sESI-MS mix of 100ng/mL 7 Nitrosamines . 5/7 are visible in the spectrum.*
*Present: NPYR, NDEA, NPIP, NDPA, NDBA | Absent: NDMA, NMEA*

# Biopharma



Schematic design of an Immunoglobulin (IgG)




**Light Chain-65.7% sequence coverage**

DIQMTQSPSTLSASVGDRVTITCSASSRVGYMHWY
QQKPGKAPKLLIYDTSKLASGVPSRFSGSGSGTEFT
LTISSLQPDDFATYYCFQGSGYPFTFGGGTKVEIKRT
VAAPSVFIFPPSDEQLKSGTASVVCLLNNFYPREAKV
QWKVDNALQSGNSQESVTEQDSKDSTYSLSSTLTL
SKADYEKHKVYACEVTHQGLSSPVTKSFNRGEC

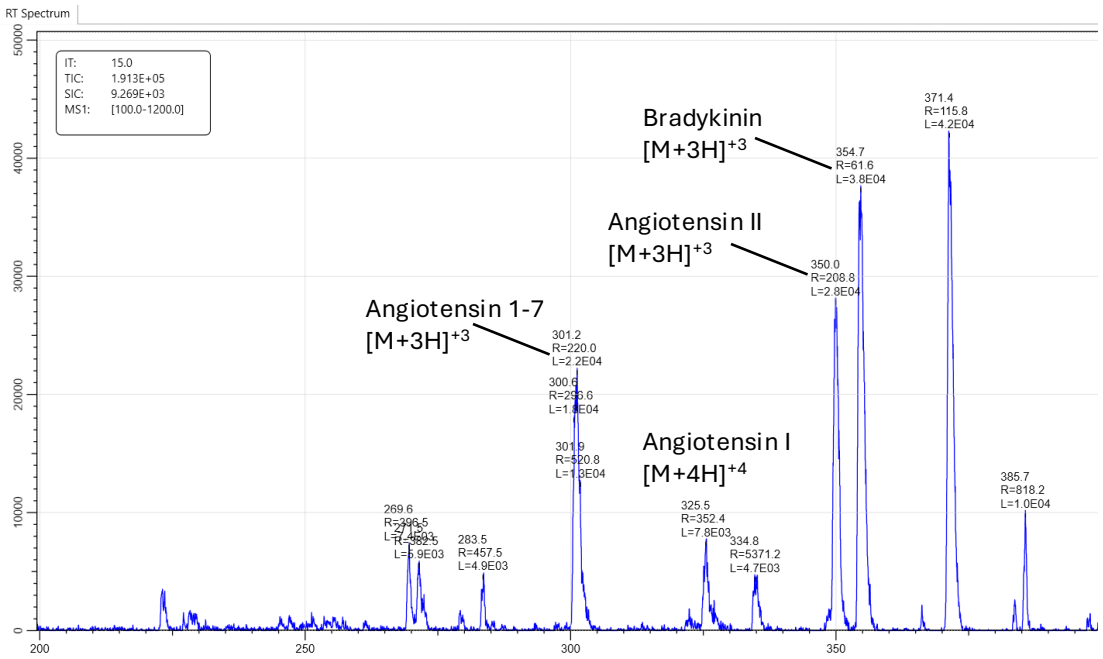
**Heavy Chain-42.3% sequence coverage**

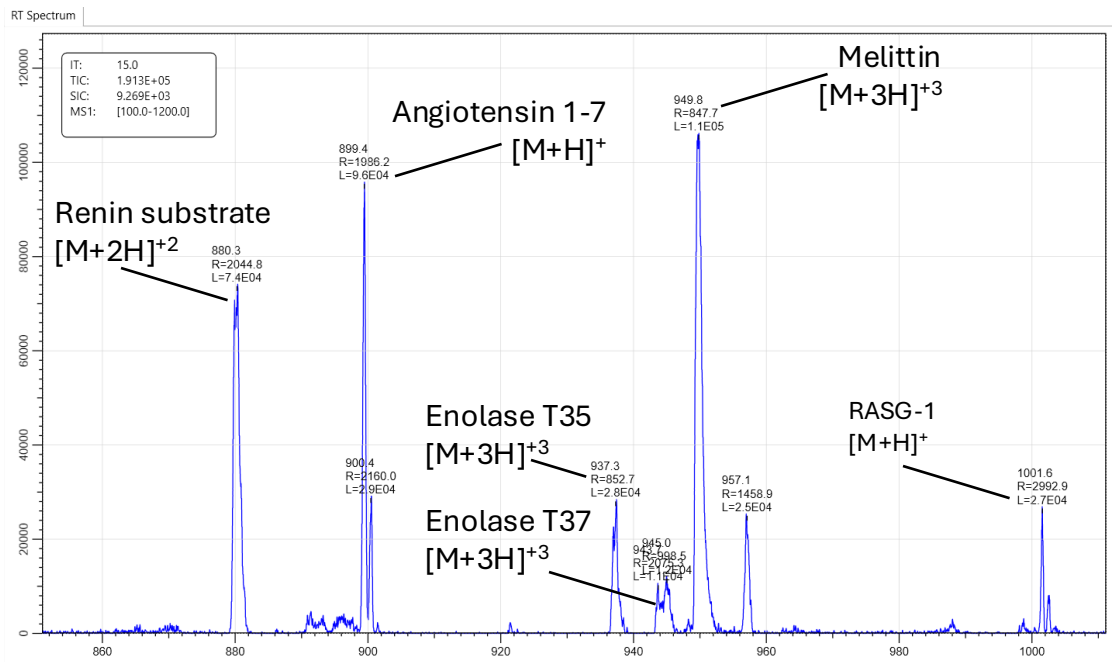
pQVTLRESGPALVKPTQTLTLTCTFSGFSLSTAGMS
VGWIRQPPGKALEWLADIWWDDKKHYNPSLKDRLTI
SKDTSKNQVVLKVTNMDPADTATYYCARDMIFNFYF
DVWGQGTTVTVSSASTKGPSVFPLAPSSKSTSGGT
AALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVLQ
SSGLYSLSSVVTVPSSSLGTQTYICNVNHKPSNTKV
DKRVEPKSCDKTHTCPPCPAPELLGGPSVFLFPPKP
KDTLMISRTPEVTCVVVDVSHEDPEVKFNWYVDGVE
VHNAKTKPREEQYNSTYRVVSVLTVLHQDWLNGKE
YKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSR
EEMTKNQVSLTCLVKGFYPSDIAVEWESNGQPENN
YKTTPPVLDSDGSFFLYSKLTVDKSRWQQGNVFSC
SVMHEALHNHYTQKSLSLSPG

ESI-MS of NIST mAb Trypsin Digest for Mass Range (35-1250 Da)

# Biopharma

ESI-MS of Waters MassPrep




| | Name | Molecular Weight (g/mol) | Peaks, m/z | | | | |
|---|---|---|---|---|---|---|---|
| | | | $[M+H]^+$ | $[M+2H]^{+2}$ | $[M+3H]^{+3}$ | $[M+4H]^{+4}$ | $[M+5H]^{+5}$ |
| 1 | Allantoin | 158.044 | 159.05 | | | | |
| 2 | RASG-1 | 1000.494 | 1001.50 | 501.25 | | | |
| 3 | Angiotensin 1-7 | 898.4661 | 899.47 | 450.24 | 300.49 | 225.62 | |
| 4 | Bradykinin | 1059.5613 | 1060.56 | 530.78 | 354.19 | 265.89 | 212.92 |
| 5 | Angiotensin II | 1045.5345 | 1046.54 | 523.77 | 349.51 | 262.39 | 210.11 |
| 6 | Angiotensin I | 1295.6775 | 1296.68 | 648.84 | 432.89 | 324.92 | 260.14 |
| 7 | Renin substrate | 1757.9253 | 1758.93 | 879.97 | 586.98 | 440.48 | 352.59 |
| 8 | Enolase T35 | 1871.9604 | 1872.96 | 936.98 | 624.99 | 468.99 | 375.40 |
| 9 | Enolase T37 | 2827.2806 | 2828.28 | 1414.64 | 943.43 | 707.82 | 566.46 |
| 10 | Melittin | 2845.7381 | 2846.74 | 1423.87 | 949.58 | 712.44 | 570.15 |

*Observed peaks.*