

THIS "COLLECTION" OF IBF DATA

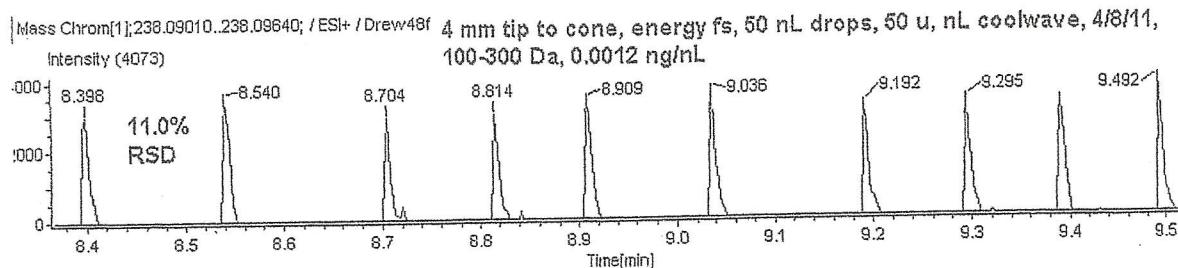
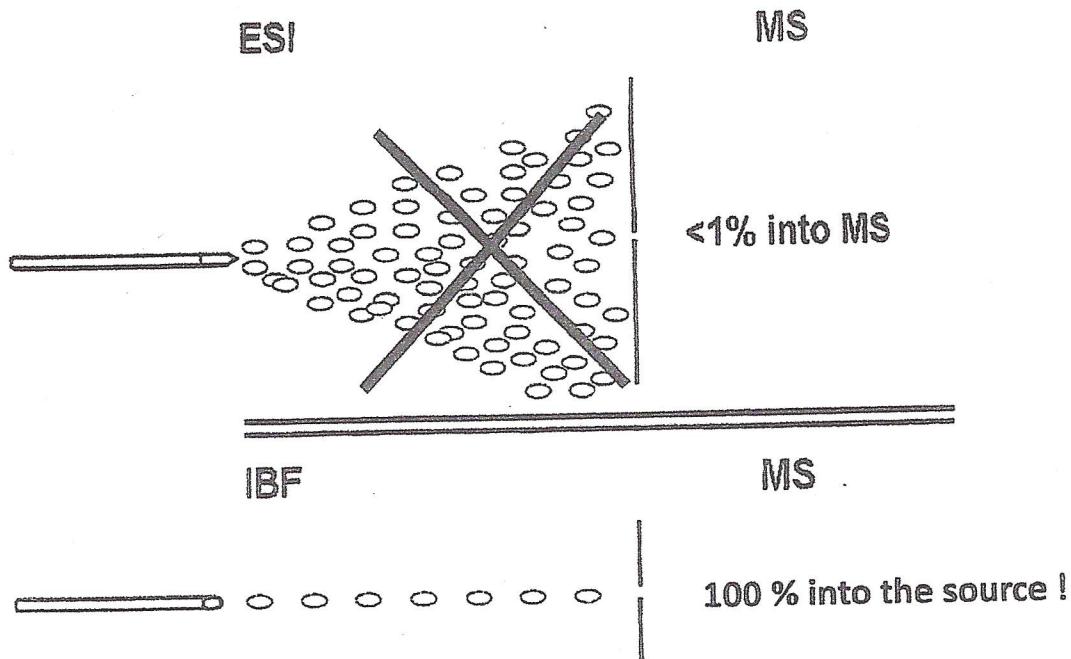
Below I show an informal collection of various spectra acquired under different conditions including equimolar alkali metals, Ag+, the ESI of coffee, the direct MS of urine with aspirin, the CMPO chelate mass spectra used to analyze Lanthanide and Actinide elements, a few proteins, peptides, oligonucleotides and nucleosides. Most data show IBF mass spectra are essentially IESI mass spectra. Consult the <http://nanoliter.com/references2017.pdf> for conditions and for the references and credits. See our many user successes, papers, & 100% "ALL IN", UPLC MS data, a world's first!

LINKS

<http://nanoliter.com/postcardjune2015no4no2.pdf>

<http://nanoliter.com/references2017.pdf>

<http://nanoliter.com/UCinasilomarposter2016.pdf>



Peak#	Time [min]	Type	Peak Width(FWHM) [min]	Area [Intens. ^ sec]	Height	Description	Start Point Time[min]	sig
23	8.398 BB		0.0072	1430.35	3006.50		8.394	2
24	8.540 BB		0.0065	1519.33	3691.90		8.533	3
25	8.704 BB		0.0056	1170.19	2942.54		8.700	1
26	8.814 BB		0.0061	1181.95	3037.00		8.806	1
27	8.909 BB		0.0066	1611.84	3602.76		8.905	4
28	9.036 BB		0.0050	1456.63	3833.80		9.032	6
29	9.192 BB		0.0055	1307.82	3330.40		9.198	2
30	9.295 BB		0.0063	1459.73	3449.67		9.291	5
31	9.390 BB		0.0074	1501.83	3375.26		9.386	-4
32	9.492 BB		0.0056	1598.34	4035.00		9.483	3

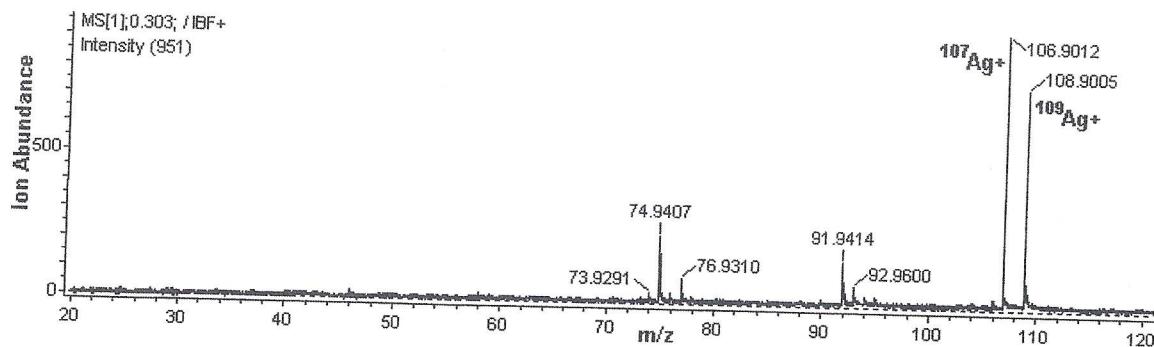


Figure 8. Mass spectrum displaying the two isotopic peaks for Ag acquired for a 100 nL drop containing 100 ng/mL of AgNO₃. The other parameters from Figure 7 remained the same.

Ion Abundance vs Enthalpy of Hydration of Allaki Metals, After Van Dorsselaer.

In the 1990's using ESI, Van Dorsselaer et al. [19] found that the relative ion abundances of the alkali metals in an aqueous solution containing 10-5 M of each cation decreased in the order: Cs⁺ > Rb⁺ > K⁺ > Na⁺ > Li⁺, which was inversely correlated with the enthalpy of hydration for the cations. (See Table 1). To obtain the mass spectrum in Figure 9, IBF was used to shoot 100 nL drops of an acidified methanol solution containing 10-5 M of each cation into the TOF MS. The relative ion abundances for the cations listed in Table 1 obtained using IBF sample introduction show a similar trend to that observed by Van Dorsselaer using ESI and it was correlated with our initensity values with a correlation coefficient of 1.01, another indicator that IBF produced ions were essentially "ESI-like" in nature.

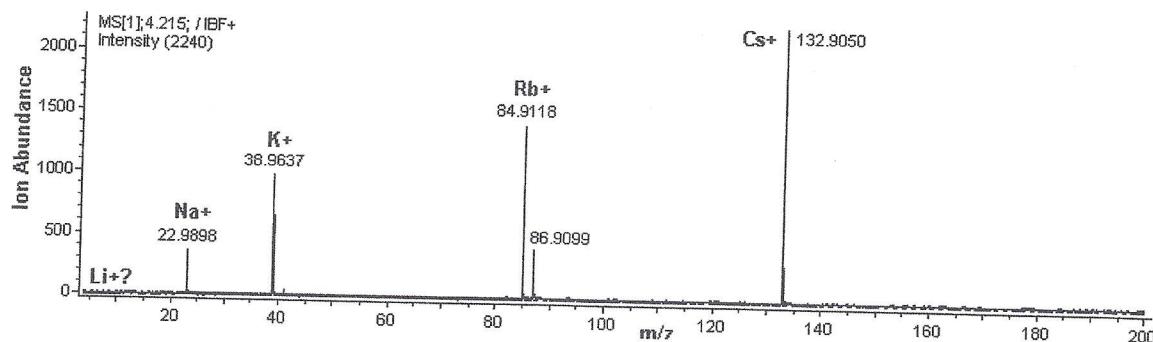
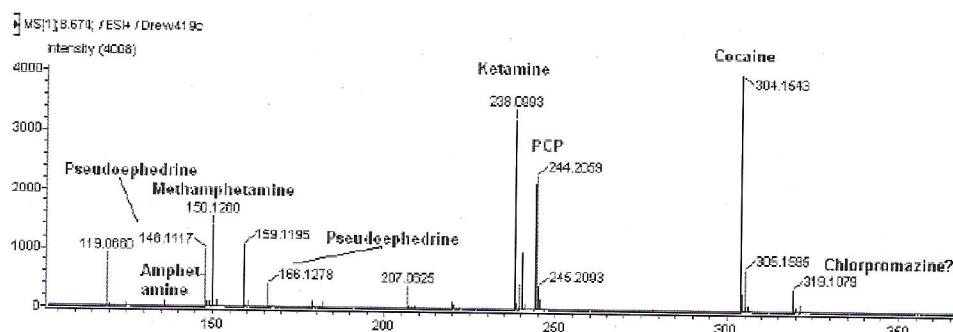
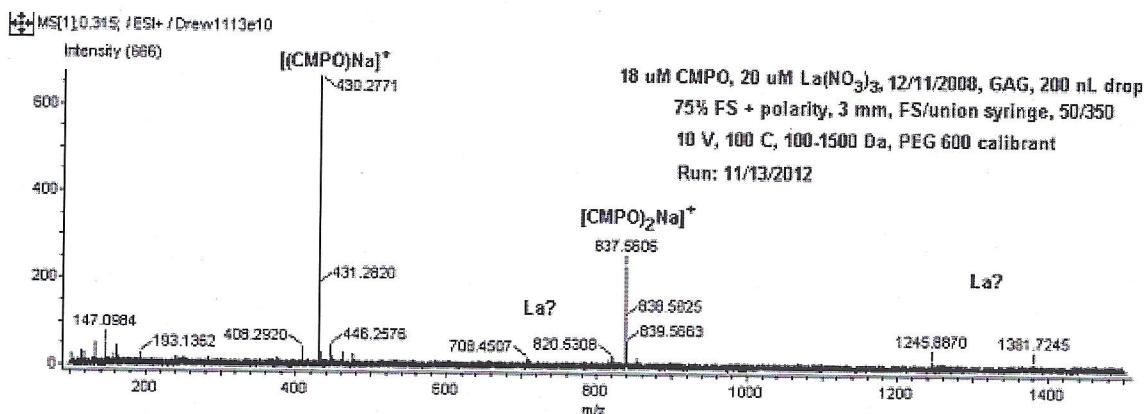


Figure 9. Composite mass spectrum of alkali metal cations. Each cation concentration in acidified methanol was 10-5 M and 100 nL drops were shot into the TOF MS. The other parameters were those for Figure 7. The mass calibration file was created from this mass spectrum.

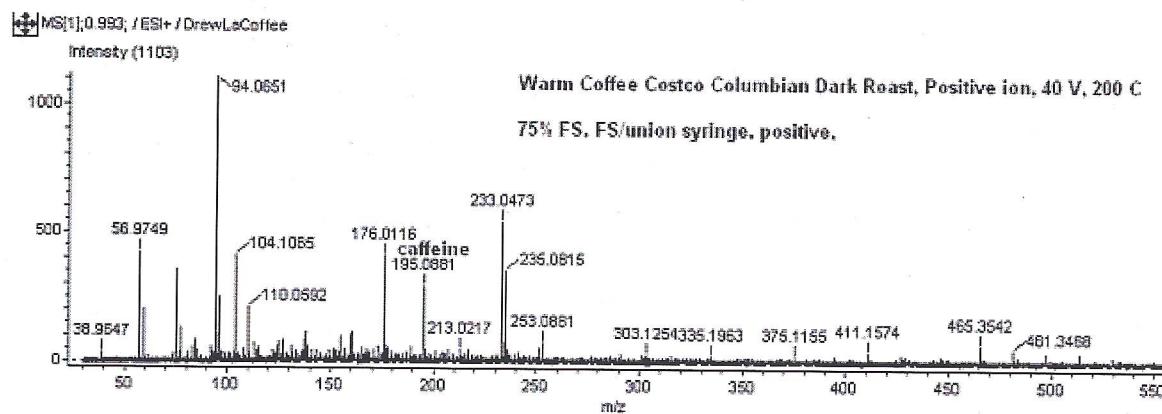
MS of mixture of drugs showing mostly ($M+H$)⁺ and collisional fragments typical of ESI.



The following MS is from a compound used to chelate radiochemicals at DOE.



The following MS was as shot as indicated, it was actually warm coffee. Caffeine identified.

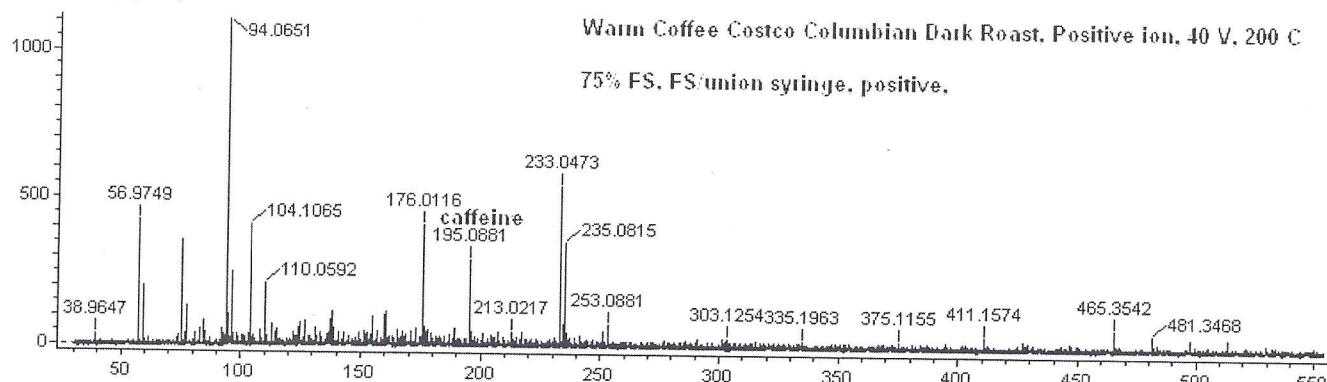


This was from an equimolar mix of alkali metals after Van Dorsselaer per previous input.

$M+H = 195$

MS[1];0.993; / ESI+ / DrewLaCoffee

Intensity (1103)



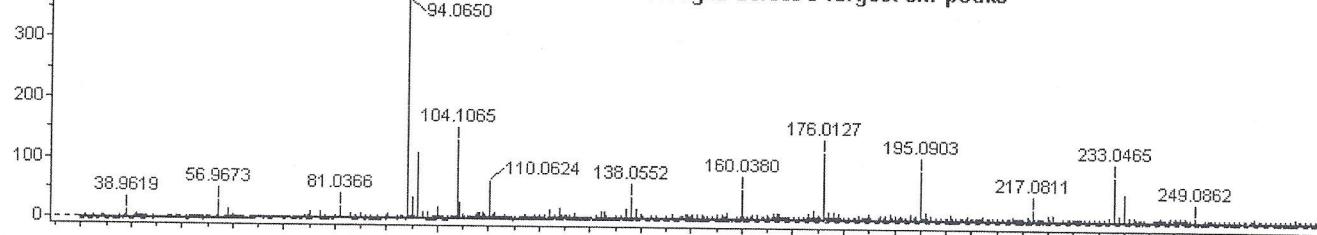
Warm Coffee Costco Columbian Dark Roast, Positive ion, 40 V, 200 C

75% FS, FS/union syringe, positive,

MS[1];0.590..0.600; / ESI+ / DrewLaCoffee

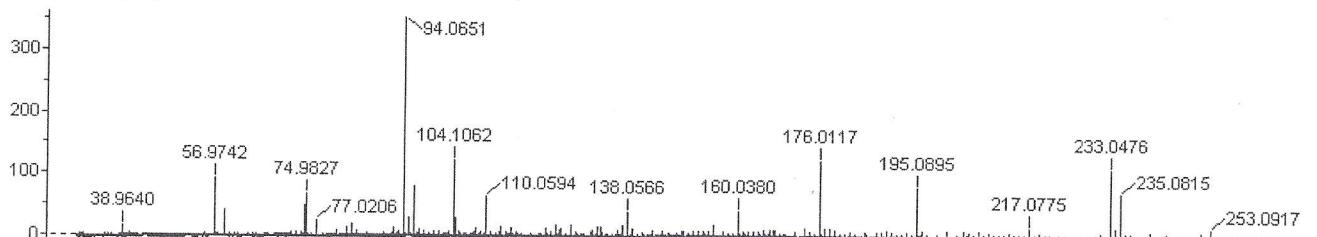
Intensity (367)

Averages across 3 largest chr peaks



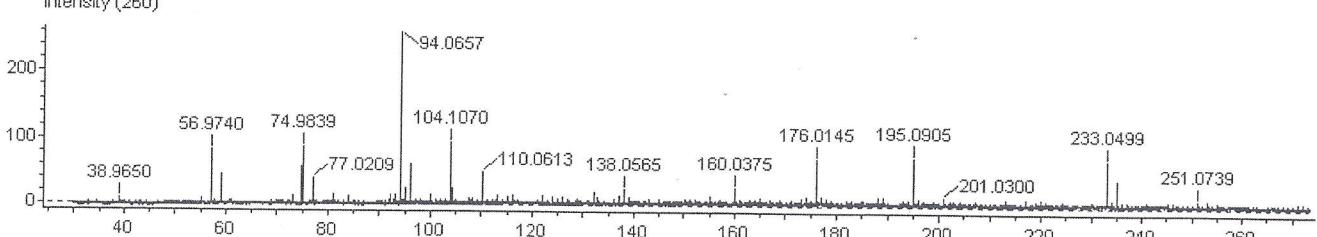
MS[1];0.991..1.002; / ESI+ / DrewLaCoffee

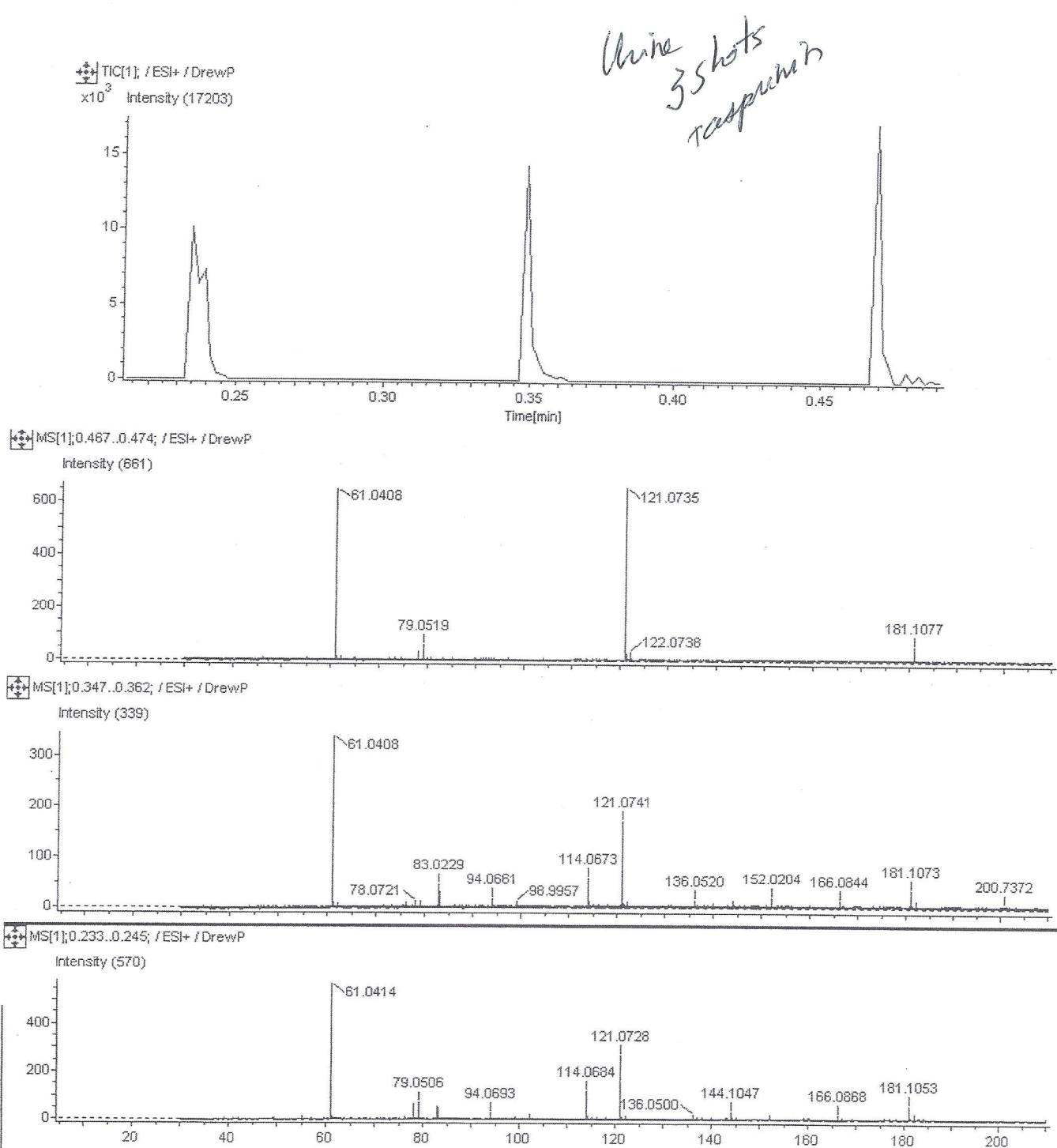
Intensity (355)



MS[1];1.066..1.099; / ESI+ / DrewLaCoffee

Intensity (260)





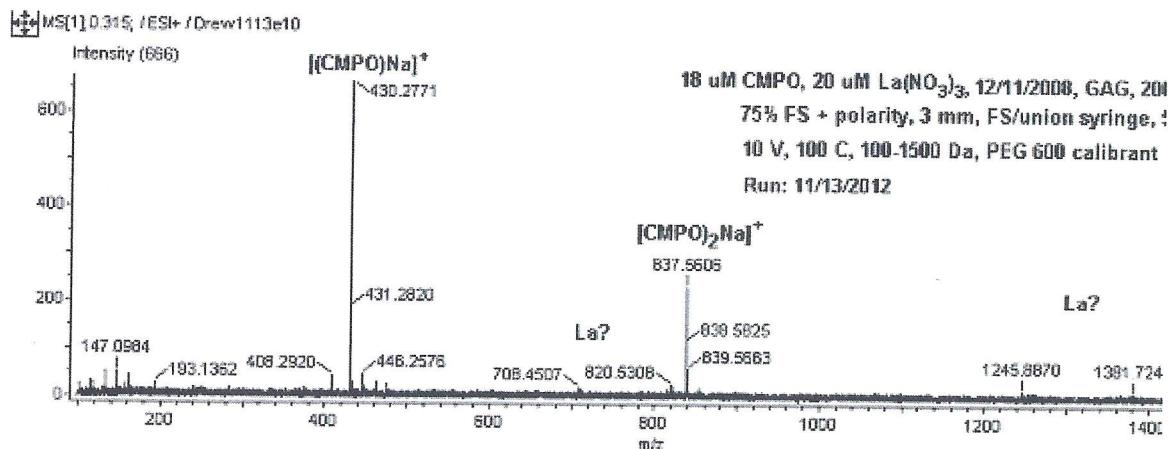
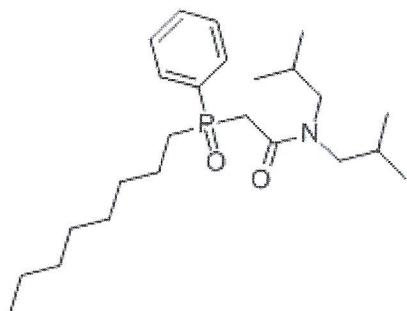
bla?

As pun?

Unre

The following MS is from a compound used to chelate radiochemicals at DOE.

Octyl(phenyl)-N,N-diisobutylcarbamoylmethylphosphine oxide



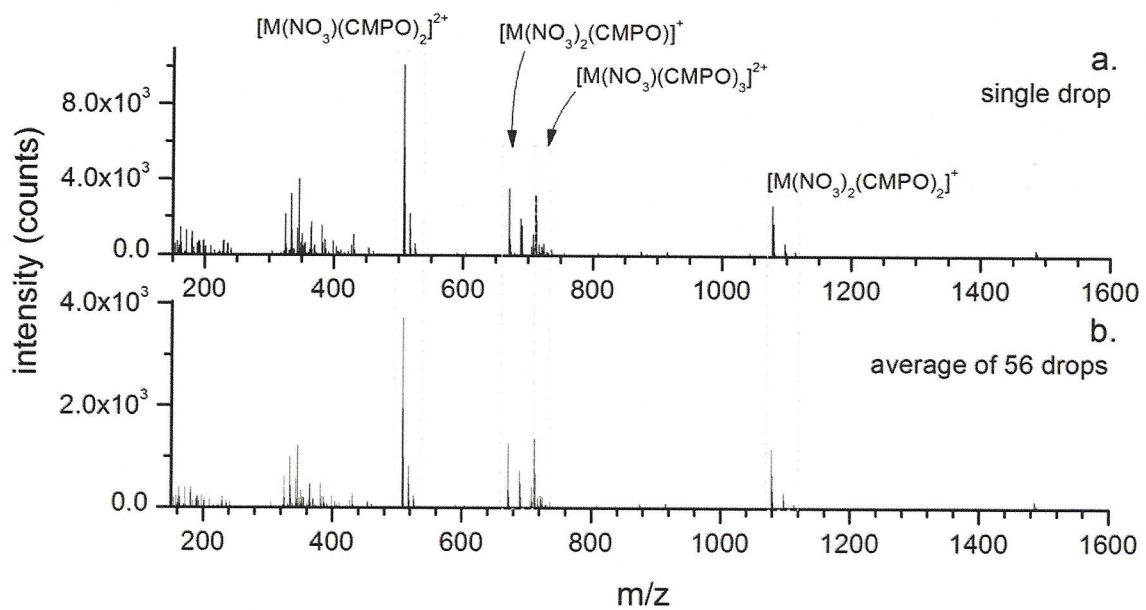
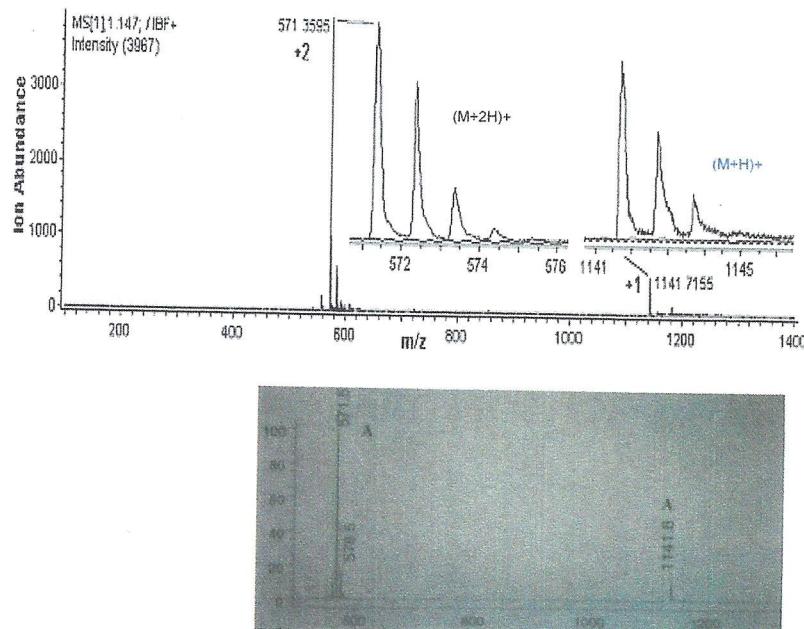
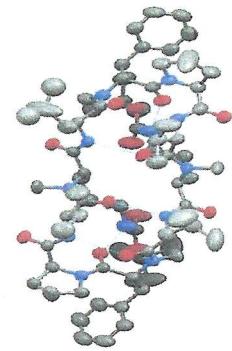


Figure 5. Positive ion spectra of a solution of Ce, Tb, and Lu nitrates with CMPO.

Can IBF do proteins, peptides, e.g., Gramacidin S as well as organics, inorganics?



Formula C₆₀H₉₂N₁₂O₁₀
Mol. Mass = 1140.7059



Comparison of intensities between doubly charged ions $[M + 2H]^{2+}$ and singly charged ions $[M + H]^+$ of gramicidin S by electrospray mass spectrometry.
Suzan M. Yerpe et al.

Source
Central Research Laboratory, Hitachi Ltd., Tokyo, Japan.

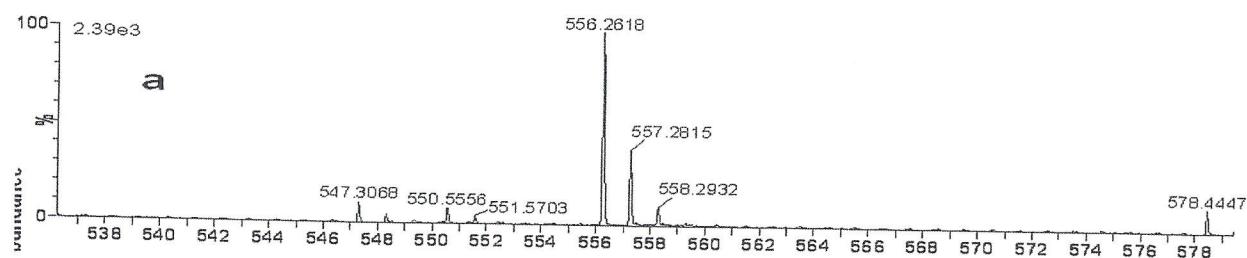
Abstract
The reason why the intensity of doubly charged ions $[M + 2H]^{2+}$ of gramicidin S is higher than that of singly charged ions $[M + H]^+$ in electrospray is investigated by ion evaporation theory. As a result of computation of the total free energies of extracting $[M + 2H]^{2+}$ and $[M + H]^+$ from a charged droplet to infinity, it is found that the total free energy of $[M + 2H]^{2+}$ is estimated to be lower than that of $[M + H]^+$. This clearly supports the experimental result. In addition, the importance of the electrostatic contribution in electrospray is demonstrated by showing the result that the total free energy of $[M + 2H]^{2+}$ without electrostatic contribution is higher than that of $[M + H]^+$.

HP 1100 MSDESI Spec Gramacidin S from V. Shakkottai, et al.
J. Peptide Res., 2002, 60, 112-120. Used with permission.

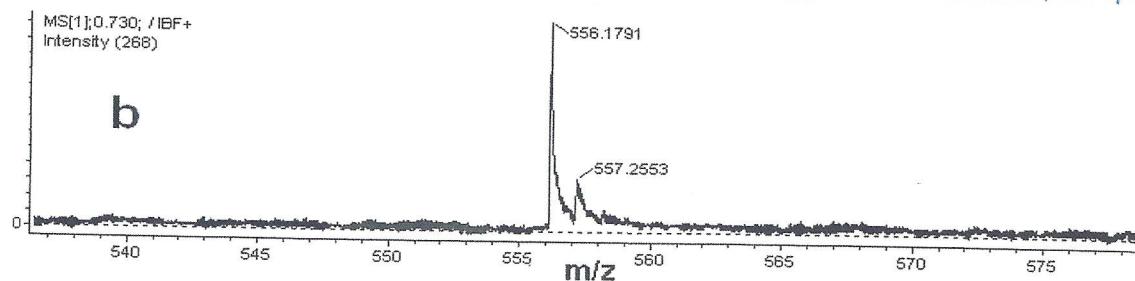
YES, IBF on a JEOL TOF looks here like ESI on an HP 1100

First comparison of IBF MS on Two Different Instruments. Spec's Similar. ESI like.

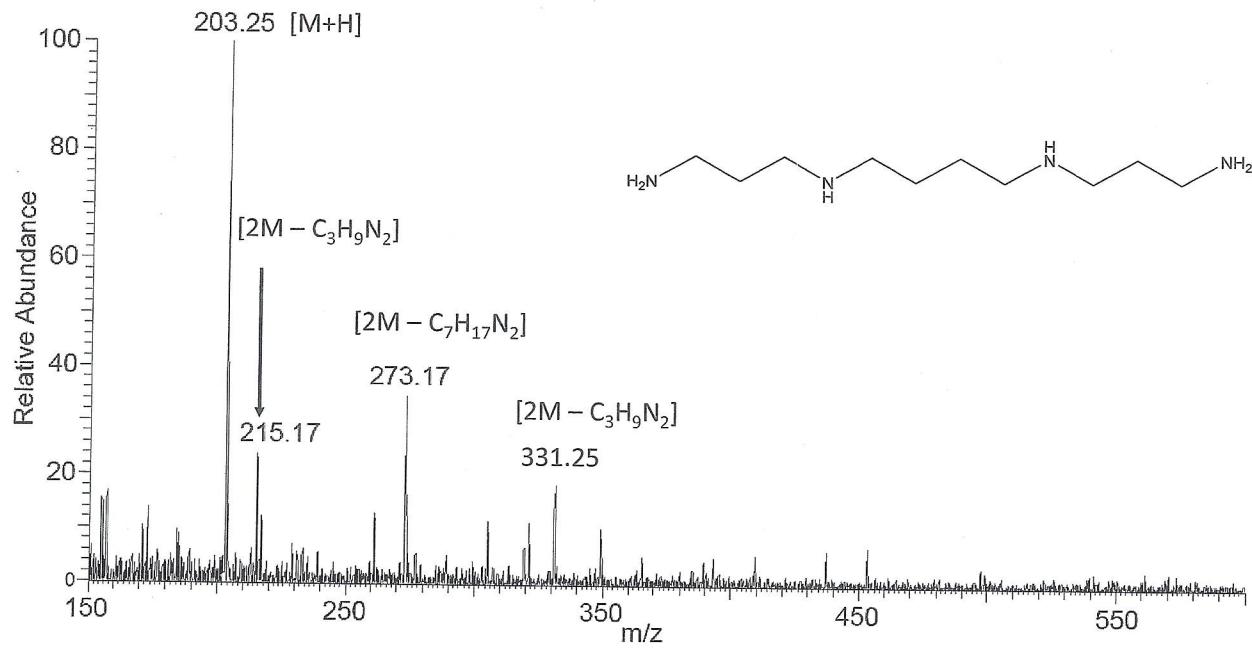
Leucine enkaphalin, YGGFL, on Waters Premier Q TOF, IBF MS, Summed, 100 pg, NH₄OAC.



Leucine enkaphalin, YGGFL, JEOL TOF, IBF MS, Single spectrum, 20 pg, HCOOH, res 5800, not optimized.



Positive Ion Mode
250 nM spermine delivered at 100 nLs
202.3



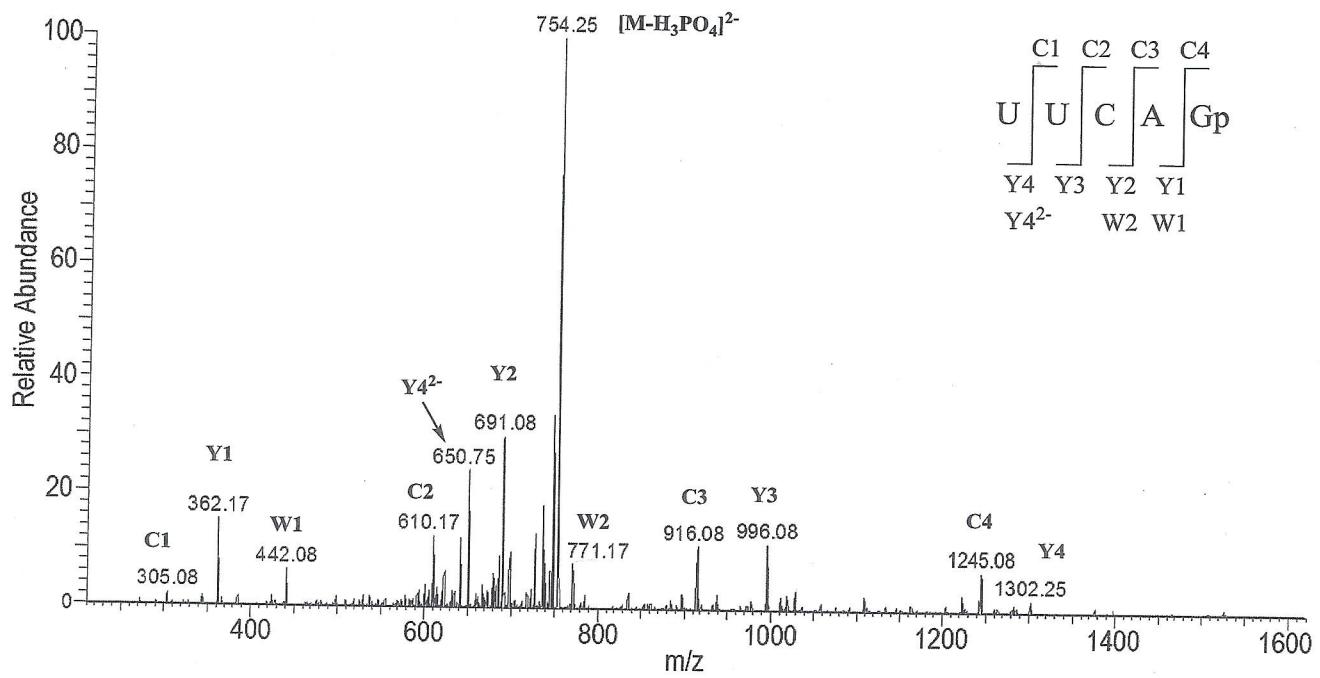
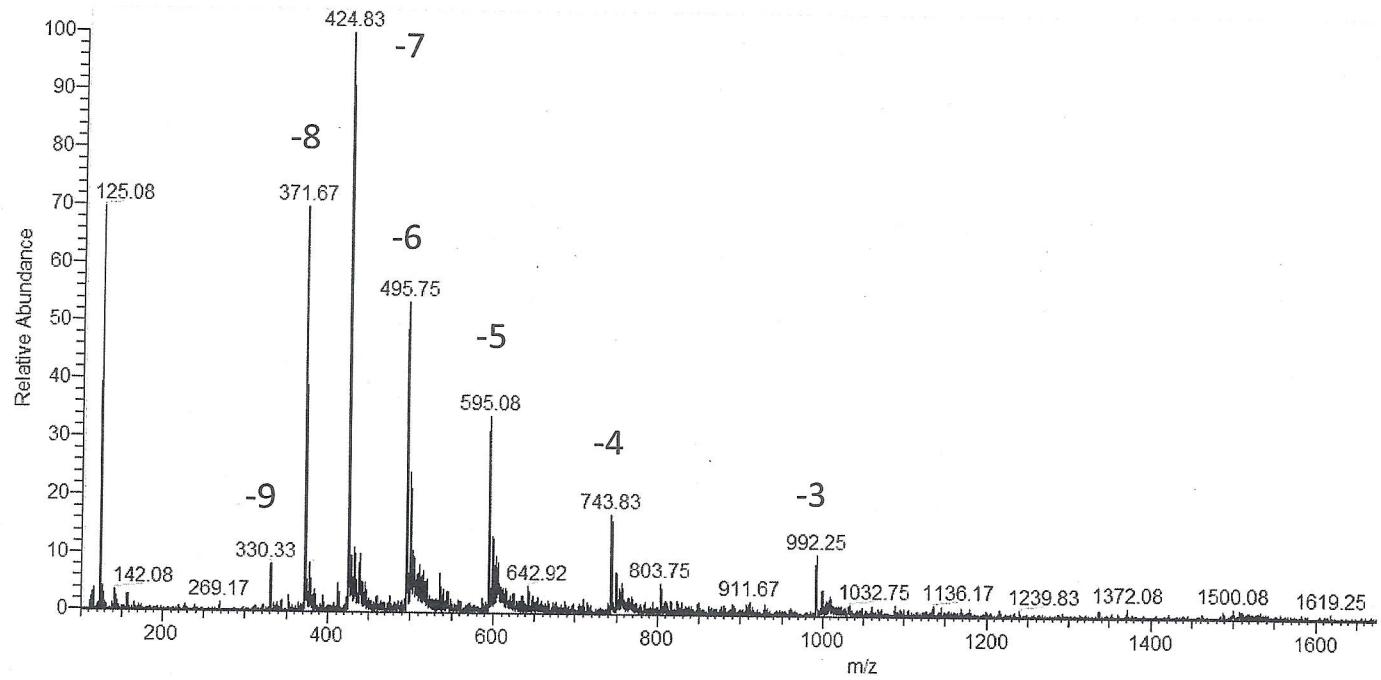


Figure 4. Collision induced dissociation chromatogram of digestion product UUCAGp using IBF ionization

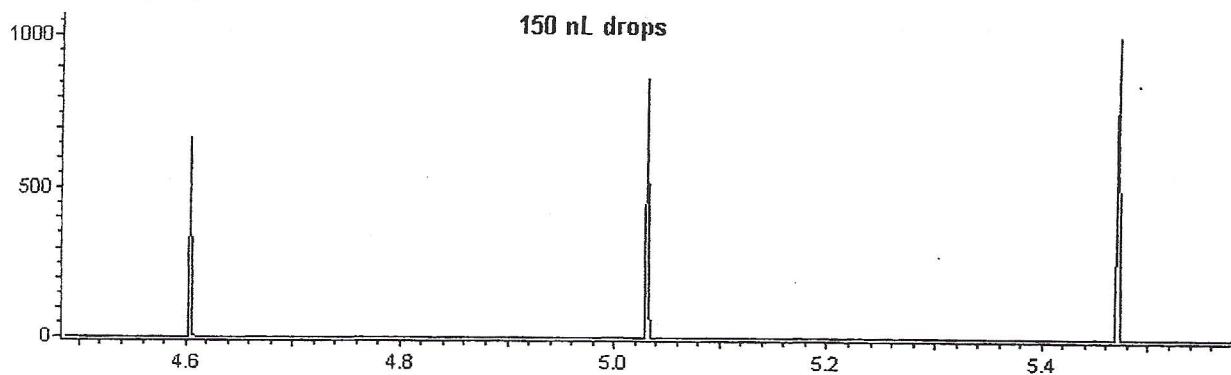
Negative Ion Mode
100 pmol dT(10) delivered at 100 nLs



TIC[1]; / ESI+ / CheekA
Intensity (1058)

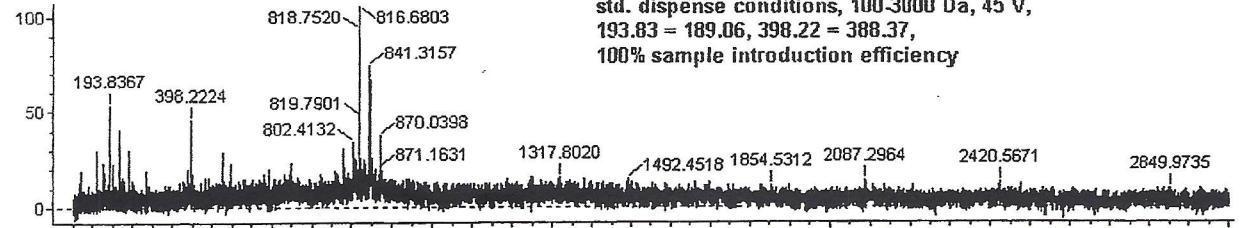
Mouth scrapings in ACN and formic acid

150 nL drops

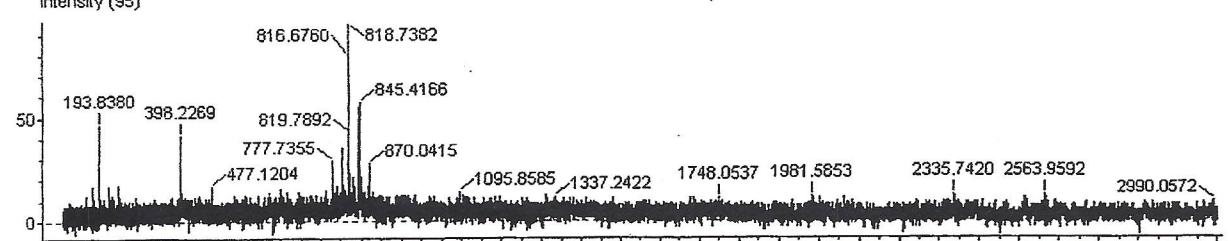


MS[1];0.990..0.991; / ESI+ / CheekNeut
Intensity (106)

Mouth scrapings in ACN only, 150 nL drops,
std. dispense conditions, 100-3000 Da, 45 V,
 $193.83 = 189.06$, $398.22 = 388.37$,
100% sample introduction efficiency



MS[1];1.439..1.440; / ESI+ / CheekNeut
Intensity (95)



MS[1];1.688; / ESI+ / CheekNeut
Intensity (80)

