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
4 mm tip to cone, energy fs, 50 nl drops, 60 u, nl coolant, 4/8/11, 100-300 Da, 0.0012 ng/ml

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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 Allalki 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 intensity 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 Dorsseleau per previous input.
Warm Coffee Costco Columbian Dark Roast, Positive Ion, 40 V, 200 C
75% MS, FS union syringe, positive.

Averages across 3 largest chr peaks
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 C60 H92 N12 O10**
Mol. Mass = 1140.7059

Comparisons of intensities between doubly charged ions ([M + 2H]+ and singly charged ion [M + H]+ of Gramacidin S by electrospray mass spectrometry.

*Source*
Central Research Laboratories, Hitachi Ltd., Tokyo, Japan

**Abstract**
The reason why the intensity of doubly charged ions [M + 2H]+ of Gramacidin S is higher than that of singly charged ion [M + H]+ is explained by ion evaporation theory. As a result of calculation between the total free energies of evaporating [M + 2H]+ and [M + H]+ from a charged ion, it is found that the total free energy of [M + 2H]+ is lower than that of [M + H]+. Thus, it clearly supports the experimental results. The importance of the electronic contribution in electrospray is demonstrated by showing the result that the total free energy of [M + 2H]+ with electronic contribution is higher than that of [M + H]+.


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

203.25 [M+H]

[2M – C₃H₉N₂]

[2M – C₇H₁₇N₂]

215.17

273.17

[2M – C₃H₉N₂]

331.25
Figure 4. Collision induced dissociation chromatogram of digestion product UUCAGp using IBF ionization.
Negative Ion Mode
100 pmol dT(10) delivered at 100 nLs
**Mouth scrapings in ACN** and formic acid

**150 nL drops**

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**MS1:** 1.39, 1.44

Mouth scrapings in ACN only, 150 nL drops, std. dispense conditions, 100-3000 Da, 45 V, 193.83, 195.98, 202.47, 388.22, 398.40, 388.37, 100% sample introduction efficiency

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**Intensity (105)**

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**Intensity (100)**

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**Intensity (95)**

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**Intensity (80)**

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