# Structural elucidation of sodium- and potassium-cationized phosphatidylcholines using electron induced dissociation

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## OVERVIEW

- **Purpose:** To better identify lipid isomers and understand EID fragmentation ion chemistry.
- **Approach:** Lipid standards were analyzed by EID using a MALDI FT-ICR MS (Bruker Daltonics).
- **Results:** The intensity ratio of fatty acid to ketene fragment ions is sensitive to the fatty acyl chain positions for $[PC+Na]^+$ and $[PC+K]^+$ ion types.
- **Significance:** EID of Na and K-cationized PCs can more easily distinguish *sn*-positional isomers compared to EID of protonated PCs.

## FRAGMENTATION NOMENCLATURE

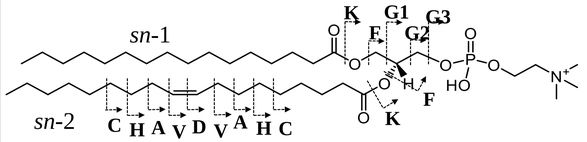


**Figure 1.** PC fragment ion nomenclature.[1]

$$\text{“X}_{n:y-z}$$

“ = the # H retained
X = Type of the cleavage
n = # of C on neutral loss
y = # of unsaturations on neutral loss
z = *sn*-position of neutral loss

| Symbol | # H retained |
|---|---|
| X | +1 H |
| ‘X | +0 H |
| “X | -1 H |
| “’X | -2 H |
| ‘X ± nH | ±n H |

## METHODS

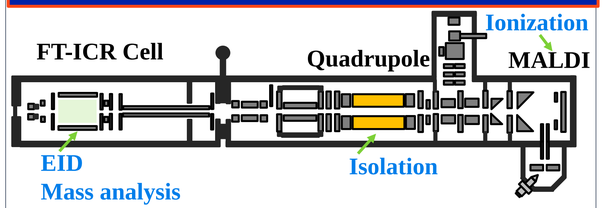


**Figure 2.** Bruker solariX FT-ICR MS. EID conditions were as follows: 23V cathode bias (EID e- energy), 35V ECD lens voltage, and 0.050s ECD pulse length.

## RESULTS

### EID of +H, +Na, and +K Ion Types for $PC_{16:0\_18:1}$ *sn*-Positional Isomers

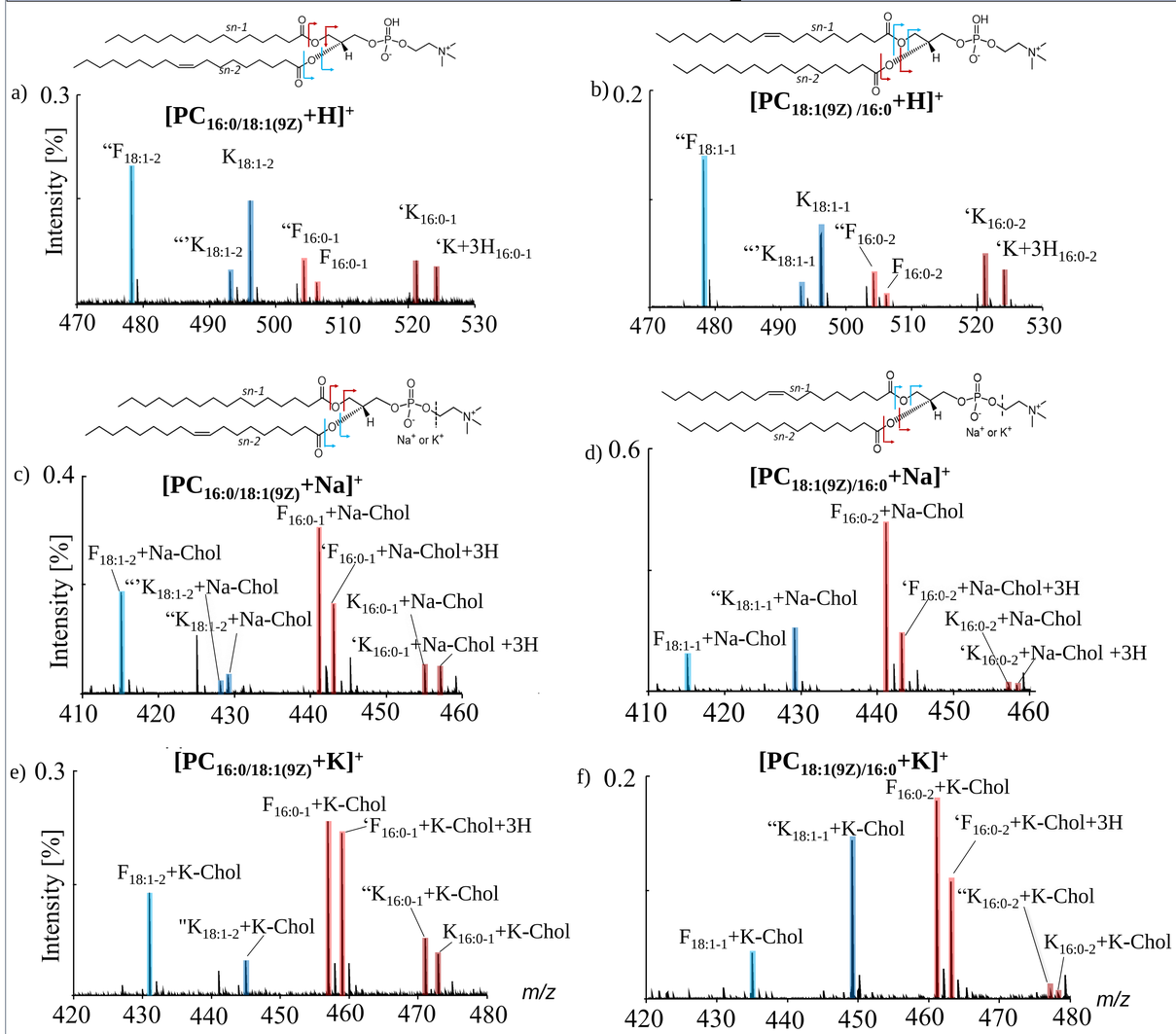


**Figure 3.** EID spectra of (a) $[PC_{16:0/18:1(9Z)}+H]^+$, (b) $[PC_{18:1(9Z)\ /16:0}+H]^+$, (c) $[PC_{16:0/18:1(9Z)}+Na]^+$, (d) $[PC_{18:1(9Z)/16:0}+Na]^+$, (e) $[PC_{16:0/18:1(9Z)}+K]^+$, and (f) $[PC_{18:1(9Z)/16:0}+K]^+$. Chol=Choline. Displayed spectra are averages of 100 spectra.

## CONCLUSIONS

- EID intensity ratio of fatty acid to ketene fragment ions for $[PC+Na]^+$ and $[PC+K]^+$ precursor ion types is more sensitive to *sn*-position than that of $[PC+H]^+$.
- EID of $[PC+Na]^+$ and $[PC+K]^+$ ion types enables facile identification of *sn*-chain isomers.
- Future work will use EID to identify $[PC+Na]^+$ and $[PC+K]^+$ ion types produced directly from the tissue in MALDI imaging mass spectrometry.

## REFERENCES

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3. JW Jones, C.J. Thompson, CL Carter, MA Kane, *Journal of Mass Spectrometry* **2015**, *50*, 1327–1339.
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