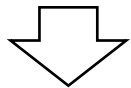


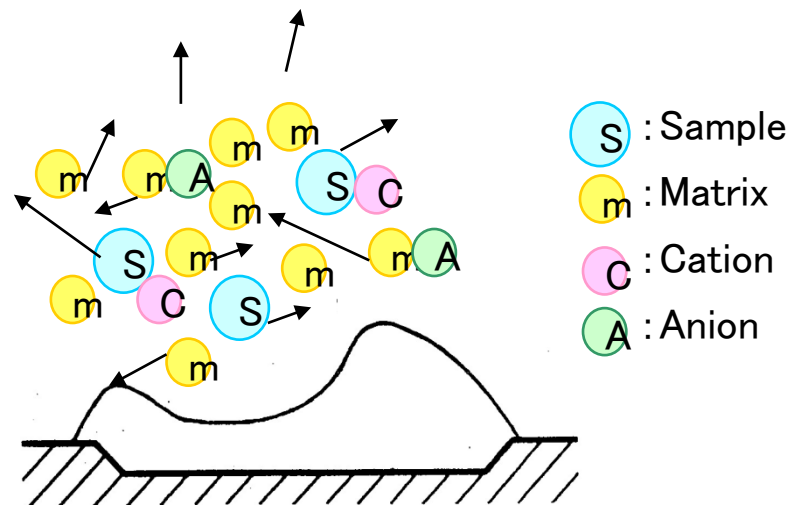
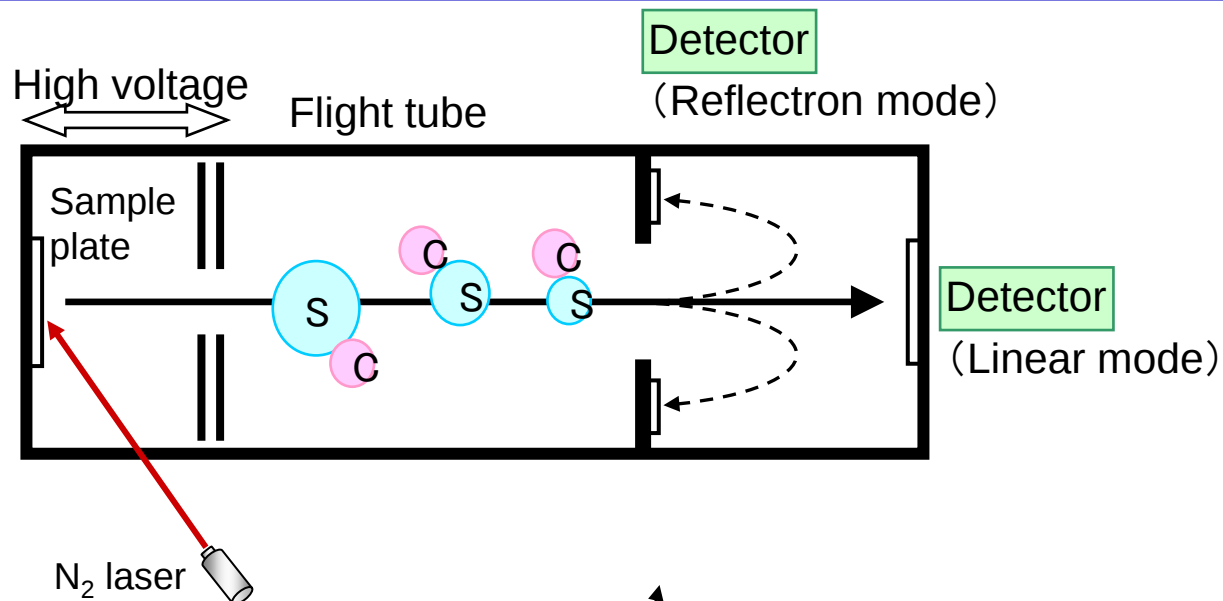
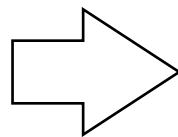
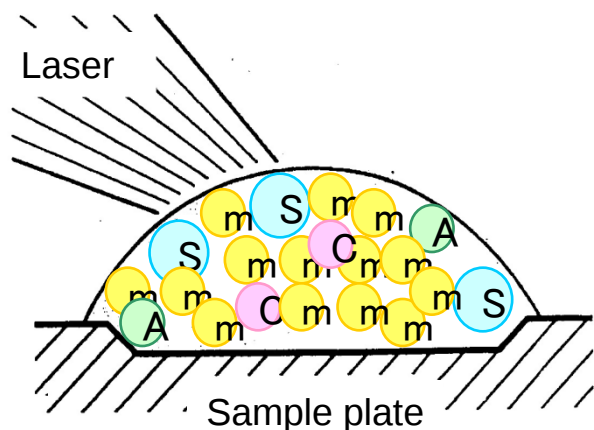
Principle of MALDI-MS

Excitation of matrix reagent
by laser irradiation



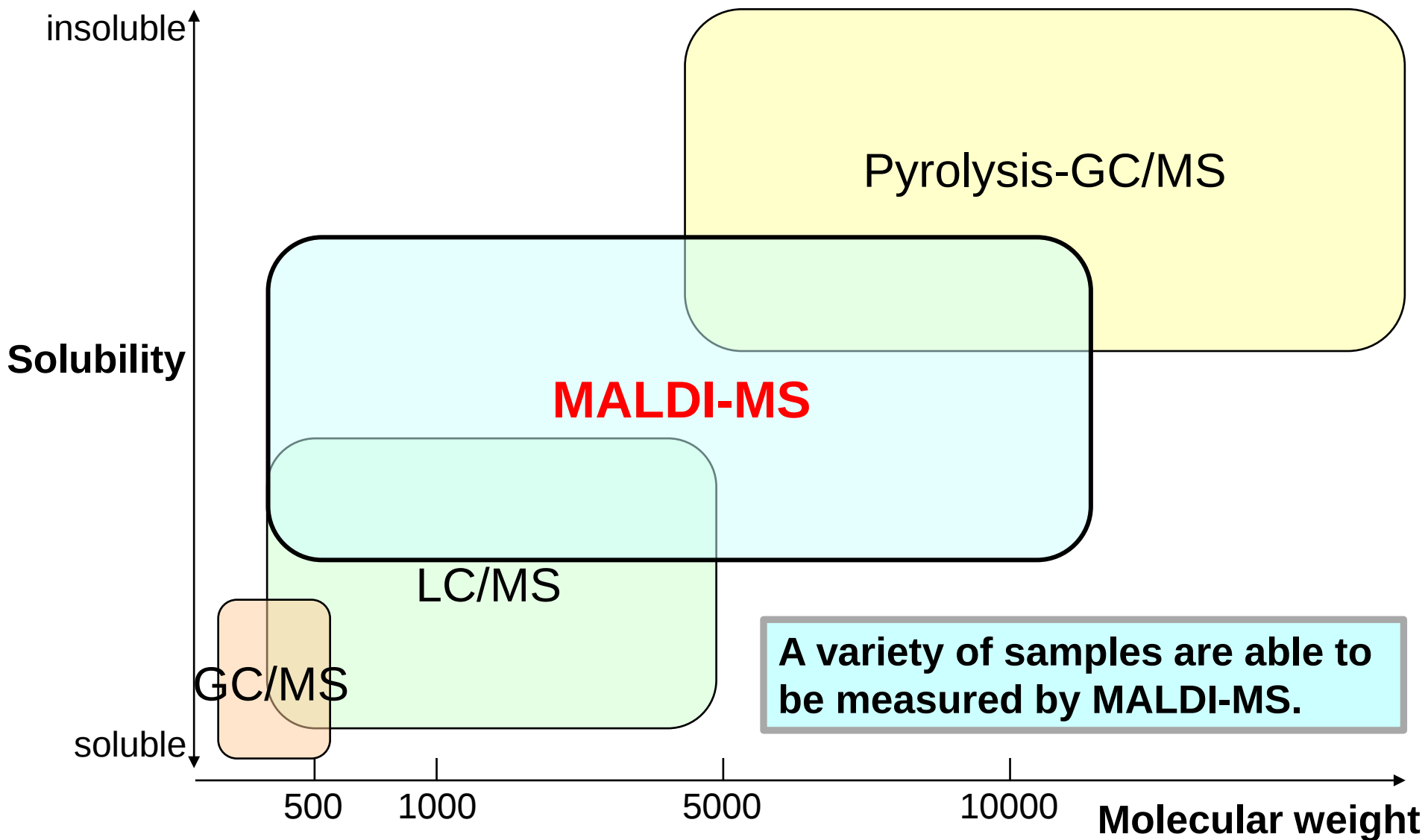
Vaporization of sample and
matrix

Ionization of sample by the
attachment of cation (proton)
to the sample molecule



S : Sample
m : Matrix
C : Cation
A : Anion

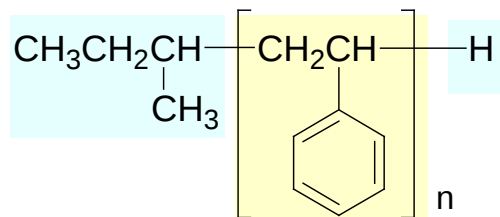
Sample classification on Mass spectrometry



Mass spectrum of Polystyrene

- High molecular weight compounds are detected as cation-adducted molecular ions ($[M+Na]^+$, $[M+Ag]^+$, etc.).
- The spectrum gives information for the molecular weights of the repeating unit and the end groups.

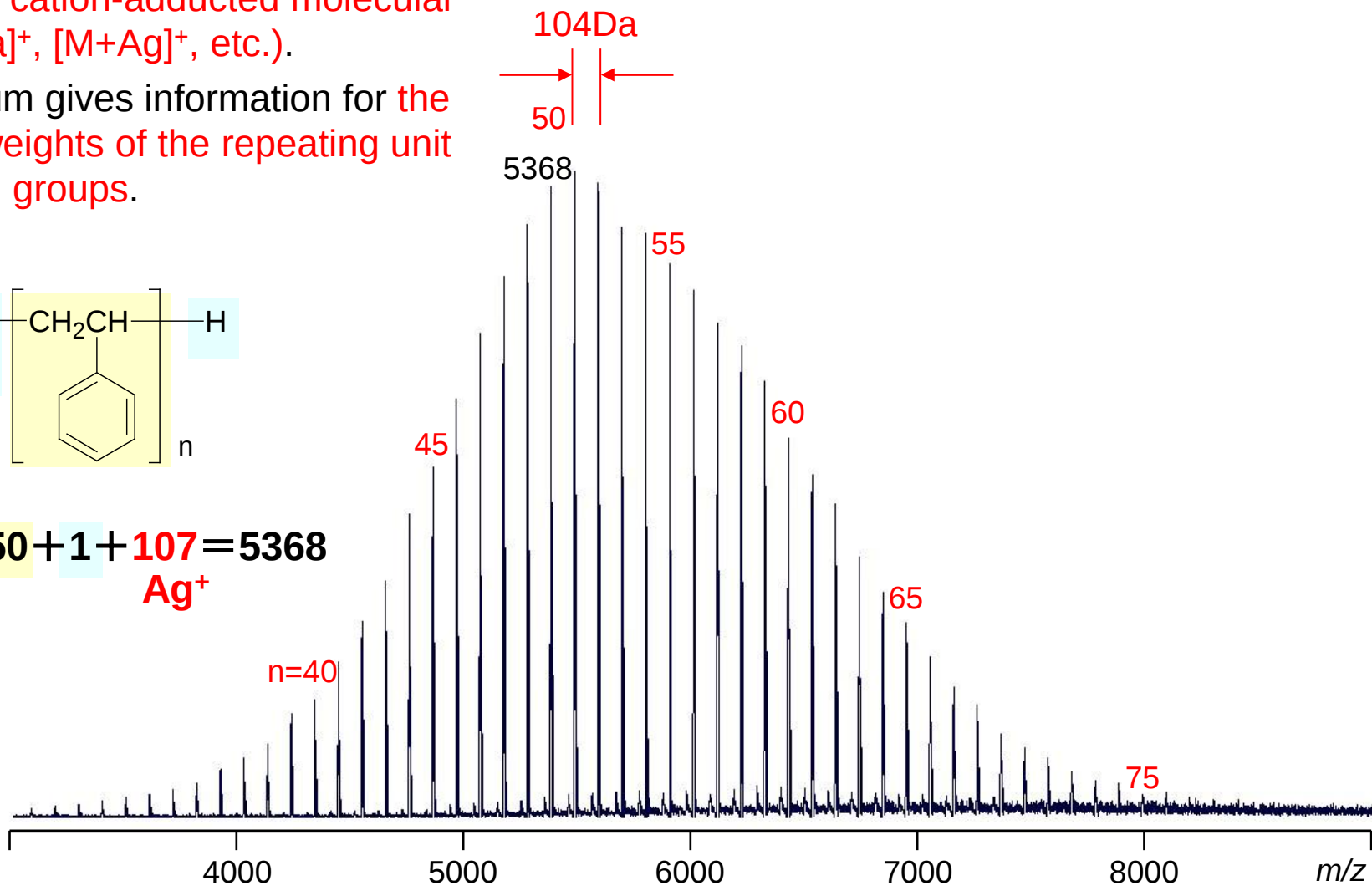
Cationization Reagent: Silver trifluoroacetate



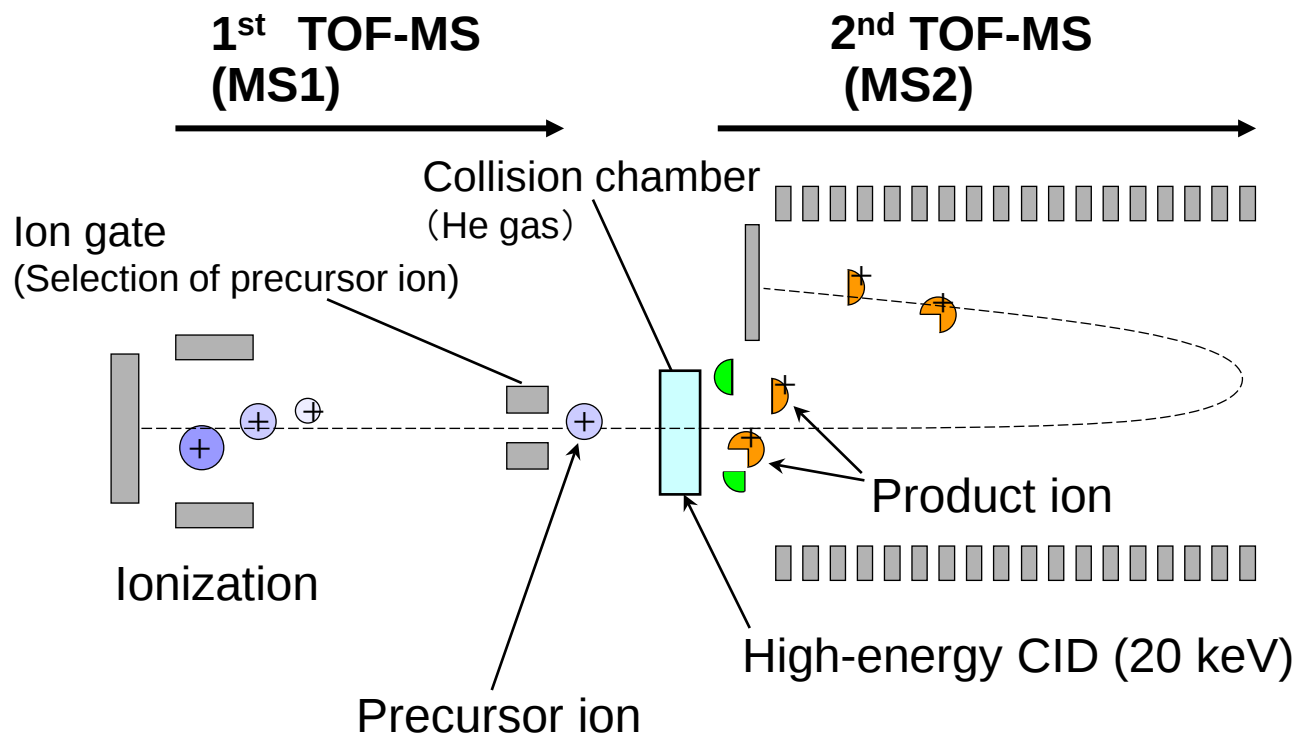
$n=50$:

$$57 + 104 \times 50 + 1 + 107 = 5368$$

Ag^+



Principle of MALDI-MS/MS (CID)



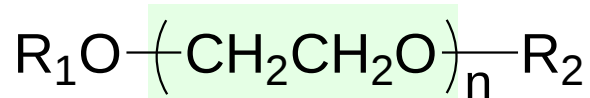
CID: Collision induced dissociation

High-energy CID produces the product ions which reflect partial structures of the compound, therefore it is possible to determine **chemical structure** of the compound.

MALDI mass spectrum of surfactant

End-modified Poly(ethylene oxide)

Cationization Reagent: Sodium trifluoroacetate



44Da

The sum of the masses
of end-groups (R_1O , R_2) is...

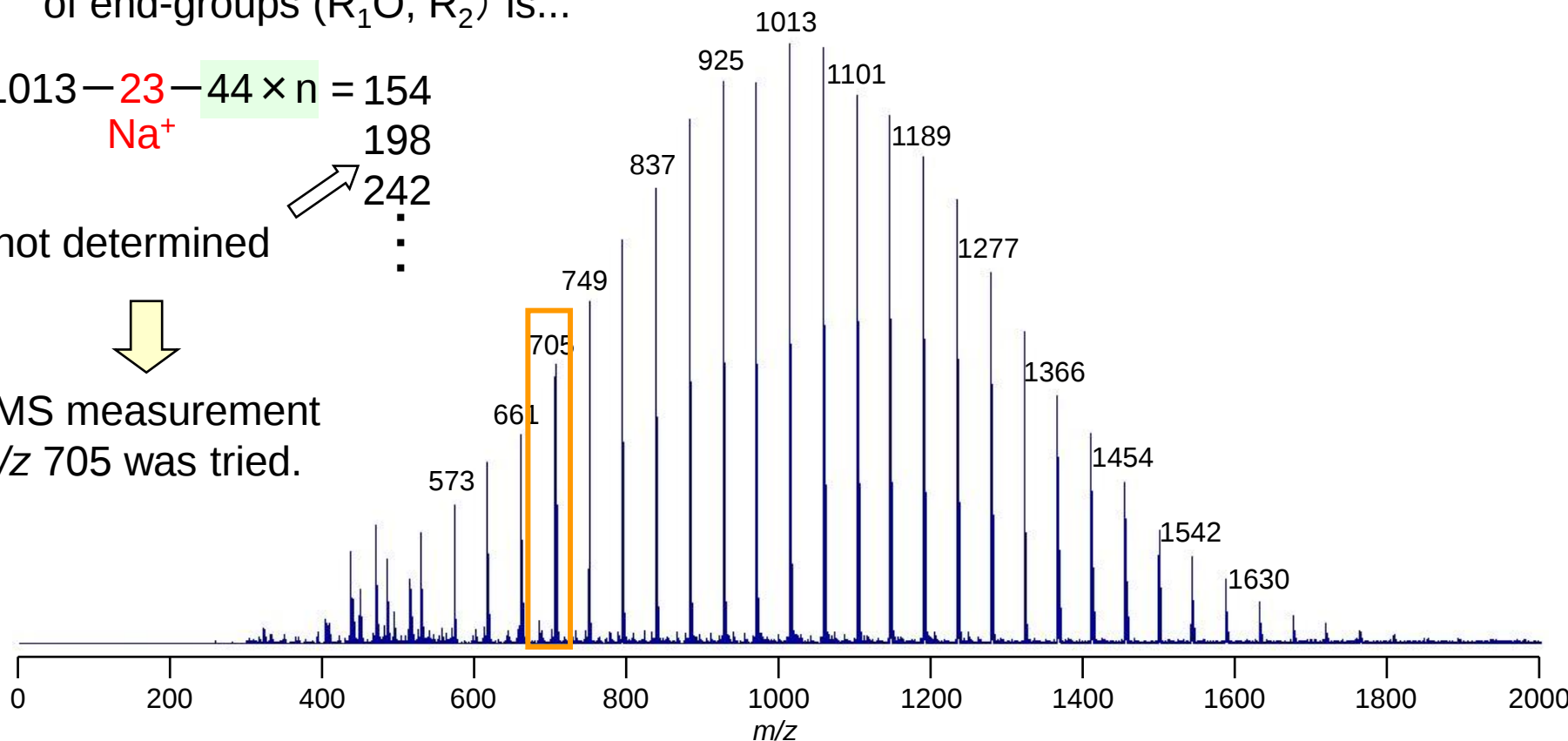
$$1013 - \text{Na}^+ - 44 \times n = 154$$

198
242
⋮

not determined

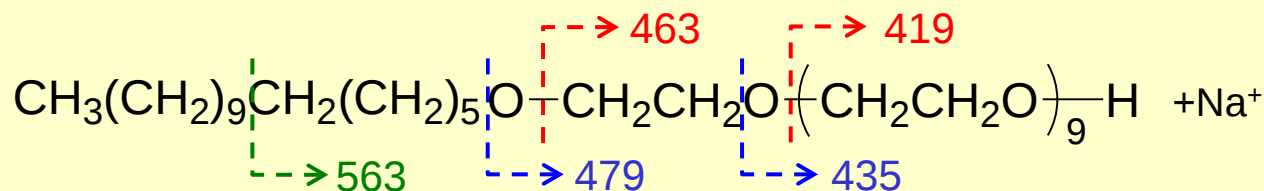


MS/MS measurement
of m/z 705 was tried.



Toray Research Center, Inc.

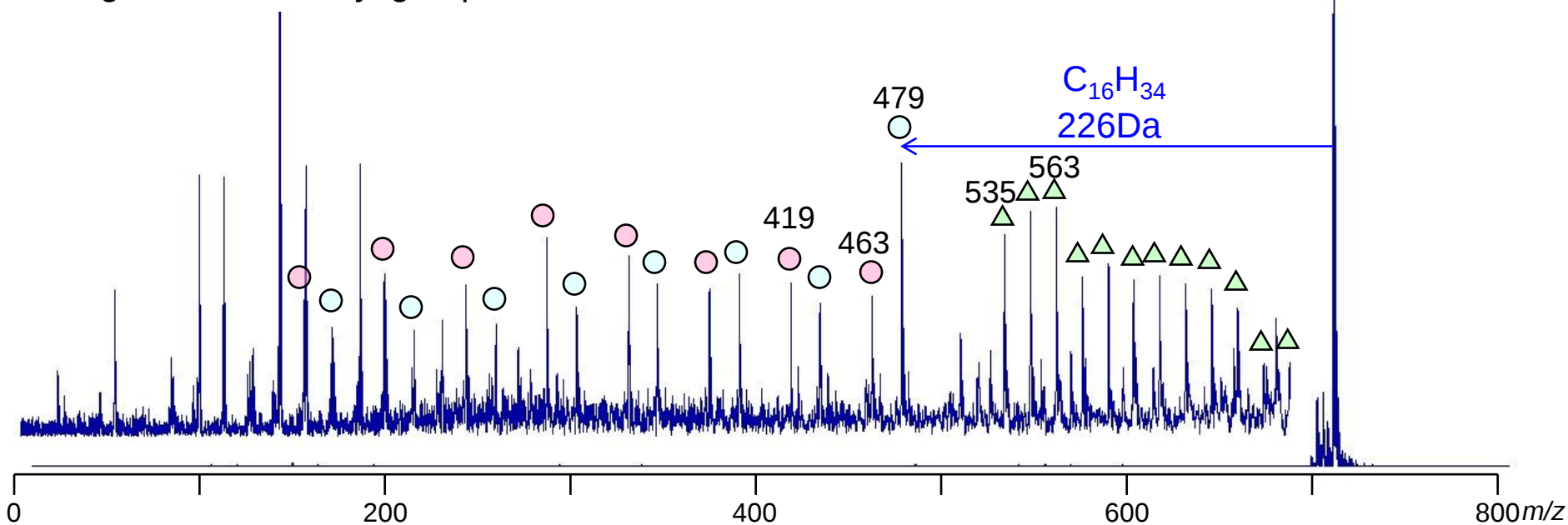
MALDI-MS/MS analysis of precursor ion (m/z 705)



PEO cetyl ether

Precursor ion
705

- : originated from PEO
- : originated from PEO
- △ : originated from Alkyl group



The information about the chemical structure is obtained by MALDI-MS/MS.