Outline

* File format
* Methods
  + High resolution MS

For standards (known Cl%, mass)

* SCCPs is mixed with lots of compounds
* Cl% effect the response factor of compounds in SCCPs
* QToF is used to collect all the ions for SCCPs
* Each ion has isotope abundances of corresponding compound
* Each ion has Cl% of corresponding compound
* Get the peaks area for those ions
* Peaks area / isotope abundances = peaks area for certain compound
* peaks area for certain compound / Cl atom = Cl normalized peak area
* Sum all the Cl normalized peak area = Cl normalized peaks area for SCCPs standards
* Cl normalized peaks area for SCCPs standards / mass = response factor
* Cl normalized peak area for certain compounds / Cl normalized peaks area for SCCPs \* compound Cl% = Cl% Contribution of certain compound
* Sum Cl% Contribution of certain compound = calculated Cl% for SCCPs standards
* Get the calculated Cl% and response factors
* Run standards with different Cl% and get their response factors
* Regression analysis with Cl% and their response factors(Cl normalized to get rid of the effects from different numbers of Cl atoms in certain compounds) to get the linear model for samples

For samples (unknown Cl%, unknown mass)

* Same way to collect the data as in standards
* Get the calculated Cl% and Cl normalized peaks area for SCCPs
* Use the standards regression model to get the response factor of this sample
* Use Cl normalized peaks area for SCCPs to get the mass of SCCPs in the sample

                       This method need to know the Cl% in the standards (actually mixture) and actually could employ internal standards and calibration curve for quantitative analysis. In high-resolution MS, we could use exact mass to stand for individual compounds.

* Low resolution MS
  + Principles

Similar to HRMS,However, in low-resolution MS, the mass would be a mixture of different compounds. According to Zeng Lixi’s work, use the isotope pattern ratio in one nominal mass could decompose the peak area into different part, which make it possible to get the contribution of different compounds.

* Input
  + Standards with known %Cl and amounts
  + Samples
* Output
  + Composition of isomers
  + Amounts
  + Calibration
  + Figures
  + Tables
  + Comparisons
* Parameters
  + Peak integration
  + Ppm of high-resolution

First, extract the SIM of ions. Then calculate RF and %Cl. Then use regression model to get the amounts and composition of isomers.

For lower resolution mass spectrum, use linear model to decompose the data before calculate the RF