Supplemented material No.1: The flowchart of the AIA calculation

**Input of the overlapping GC/MS signal**

\[ X_{\text{m:n}} = [x_1, x_2, \cdots, x_m]^T = \left[ x_{11}, x_{12}, \cdots, x_{1n} \right] \]

\[ \left[ x_{21}, x_{22}, \cdots, x_{2n} \right] \]

\[ \vdots \]

\[ x_{m1}, x_{m2}, \cdots, x_{mn} \]

\( m \): scan number (sample number in retention time); \( n \): number of mass to charge

**Set of the initial number of ICs**

\( d = 1 \)

**Calculate ICs (spectral information) from \( X_{\text{m:n}} \)**

Using the program of the ICA procedure, which is available from the website http://mole.imm.dtu.dk/toolbox/ica/mf/icaMF.zip, calculate the ICs from the input signal, \( X_{\text{m:n}} \), with the preset number of ICs, \( d \). The calculated ICs are stored in \( \hat{S}_{d:n} \).

\[ (X_{\text{m:n}}, d) \xrightarrow{\text{ICA}} \hat{S}_{d:n} = [\hat{s}_1, \hat{s}_2, \cdots, \hat{s}_d]^T = \left[ \hat{s}_{11}, \hat{s}_{12}, \cdots, \hat{s}_{1n} \right] \]

\[ \hat{s}_{21}, \hat{s}_{22}, \cdots, \hat{s}_{2n} \]

\[ \vdots \]

\[ \hat{s}_{d1}, \hat{s}_{d2}, \cdots, \hat{s}_{dn} \]

**Calculate the chromatographic profiles of the ICs**

Taking \( \hat{S}_{d:n} \) as antibodies (standard information) and \( x_j \) (the measured MS at retention time \( j \)) as antigen (overlapping MS to be resolved), using the program of IAA procedure (the supplemented material No.2), calculate the chromatographic intensity, \( c_j = \{c_{j,d}\} \), of the \( d \)th IC at the retention time \( j \). With all the \( c_j \) \((j = 1 \cdots m)\) s at every retention time, the chromatographic profile can be obtained.

\[ \hat{C}_{\text{m:d}} = (\hat{c}_1, \hat{c}_2, \cdots, \hat{c}_m)^T = \left[ \hat{c}_{11}, \hat{c}_{12}, \cdots, \hat{c}_{1d} \right] \]

\[ \hat{c}_{21}, \hat{c}_{22}, \cdots, \hat{c}_{2d} \]

\[ \vdots \]

\[ \hat{c}_{m1}, \hat{c}_{m2}, \cdots, \hat{c}_{md} \]

**Evaluation of the assumed number of ICs**

\[ X^{\text{rec}} = \hat{C} \hat{S}, \quad RRSSQ = \left( \sum_{i=1}^m \sum_{j=1}^n (x_{ij} - x_{ij}^{\text{rec}})^2 \right)^{1/2} \]

Minimum of \( RRSSQ \)?

**Output of the resolution results**

\( \hat{S}_{d:n} = [s_1, s_2, \cdots, s_d]^T, \hat{C}_{\text{m:d}} = [c_1, c_2, \cdots, c_m]^T, X^{\text{rec}} = \hat{C}_{\text{m:d}} \hat{S}_{d:n} \)
Supplemented material No.2: Program of the IA procedure

function [h, resi] = IA(antigen, antibody)

% antigen – the overlapping signal, in which each row is an overlapping spectrum.
% antibody – the standard information of the components, which can be obtained from
% the measurement of the reference substances, the theoretical simulations,
% or extracted by means of ICA, etc.
% h – affinity between the antibody and the antigen, in an overlapping signal,
% it corresponds to the concentrations of the multiple components.
% resi – residue between the extracted information and the antigen.

[row,col]=size(antigen);
[row1,col1]=size(antibody);
if col~=col1
    error('error');
end

feedback=zeros(1,col);
h=zeros(1,row1);
q=antibody*antibody';
for i=1:row1
    T(i,:)=antibody(i,:)/q(i,i);
end;
CN=row1;
clear row col col1 row1 q

dh=(antigen-feedback)*T';
number=0;residu=sum(dh*dh');
resi=antigen-feedback;
while sum(dh*dh')>1e-5 & number<2000
    h=h+dh/10;
    for i=1:CN
        if h(i)<0 h(i)=0; end
    end
    feedback=h*antibody;
dh=(antigen-feedback)*T';
number=number+1;
residu=sum(dh*dh');
resi=antigen-feedback;
clear mm pos
end